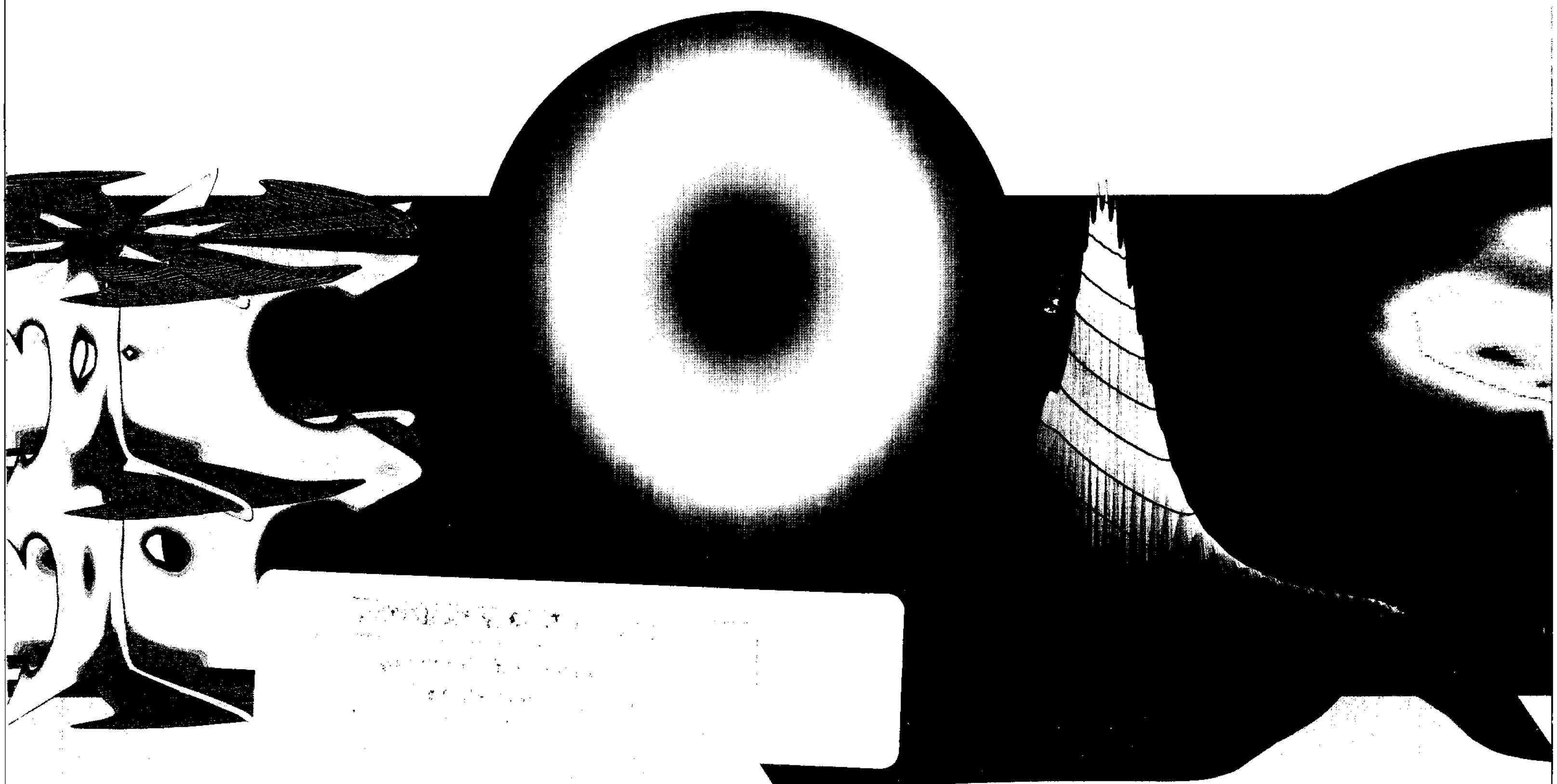
contributions to

# DoD Mission Success
## from High Performance Computing

## 1996



Computation, particularly high performance computation, has become an alternative way to find answers to scientific questions—a new tool for scientists that complements the age-old tools of analysis and experimentation. The U.S. enjoys an advantage in high performance computation capability, and our scientists and engineers are embarked on the challenge of exploiting this capability to the advantage of the warfighter.

This 1996 edition of *Contributions to DoD Mission Success from High Performance Computing* is dedicated to the leaders of the ten defense Computational Technology Areas. The vision, leadership, and hard work of these users of high performance computing are, and have been, crucial to the success of the DoD high performance computing enterprise. It is their accomplishments and those of their colleagues across the defense science, engineering and test community that are chronicled in this volume. Mission success stories were chosen to illustrate the crucial role of high performance computing at DoD laboratories, universities, and industry. For each one, the military significance of the result is highlighted.

Better understanding of and mastery of natural phenomena serve as a basis for enabling military advantage; high performance computing serves to support the search for that advantage.

Anita K. Jones
Director
Defense Research and Engineering

ADDITIONAL COPIES AND DOCUMENTATION

Additional copies of this publication may be ordered from the Defense Technical Information Center, (703) 767-8274, or by e-mail: msorders@dtic.mil

For more information about the DoD HPC Modernization Program, refer to http://www.hpcm.dren.net on the World Wide Web.

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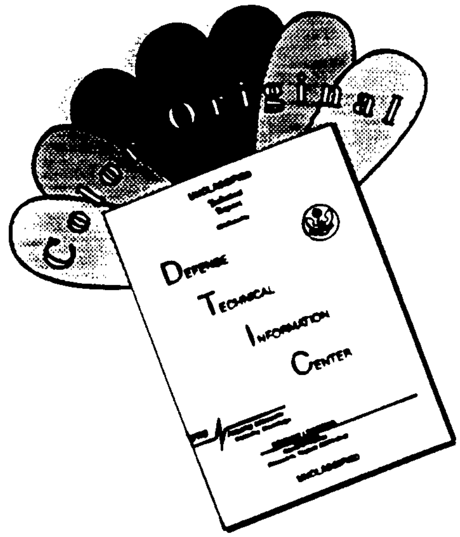


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**contributions to**

# DoD Mission Success
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# HPC Enables DoD Mission Success

# Introduction

# HPC Enables DoD Mission Success — Introduction

## HIGH PERFORMANCE COMPUTING IN DoD

High Performance Computing (HPC) has been playing and will continue to play a major role in the ability of the United States to maintain and increase its lead in the technological superiority of its warfighting systems. In the Gulf War, for example, an entirely new munition for deep penetration of enemy bunkers, the GBU-28, was designed and used in battle in a matter of weeks. HPC was critical for simulating the munition's performance. This, in turn, drove the rapid design and production process.

As DoD transitions its weapons systems design, test, and evaluation to rely much more heavily on modeling and simulation, the nation can expect many more examples of the profound effects of HPC capabilities on the technological superiority of our warfighting systems. A few representative areas in which HPC is making and will continue to make real differences in weapon systems design are imagery and signal intelligence, ocean modeling, weather prediction, airlift optimization, automatic target recognition, aircraft stores certification, and advanced communications, command and control.

Because of the importance of HPC in maintaining technological superiority, the HPC Modernization Program (HPCMP) has emerged as a key corporate DoD initiative.

## THE HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

The High Performance Computing Modernization Program is designed to support DoD research, development, test, and evaluation (RDT&E) in their quest for military advantage through better understanding and mastery of natural phenomena. Successes from this program were first reported in Contributions to DoD Mission Success from High Performance Computing — March 1995. The present publication is the second such report.

The HPC Modernization Program reports directly to the Director of Defense Research and Engineering. Its mission is to modernize the HPC capability of DoD laboratories and centers to a level comparable to the best anywhere, using commercial off-the-shelf hardware configured to meet DoD mission success requirements. The Program is a coordinated initiative to develop and sustain large HPC systems with extensive capabilities to address user requirements for hardware, software, programming environments, and training; smaller, distributed HPC centers; high-speed networks connecting users to the systems; and a scalable applications software effort to develop a set of critical multipurpose DoD applications

programs that run efficiently on new generations of scalable HPC systems. The large system capabilities are called Major Shared Resource Centers, while the smaller ones are called Distributed Centers. For more information about the Program and its centers, see the World Wide Web site at http://www.hpcm.dren.net.

## COMPUTATIONAL TECHNOLOGY AREAS

The DoD HPC user base includes almost 3,000 computational scientists and engineers at approximately 50 DoD science and technology (S&T) laboratory locations and numerous university and industry sites, and over 1,200 computational scientists, engineers, and analysts at approximately 20 developmental test and evaluation (DT&E) facilities. In order to focus the HPC Modernization Program to meet the needs of this large, diverse group, the S&T and DT&E computational workload has been categorized into ten Computational Technology Areas (CTA). They are: structural mechanics, fluid dynamics, chemistry and materials science, electromagnetics and acoustics, climate/weather/ocean modeling, signal/image processing, forces modeling and simulation/C4I, environmental quality, electronics and nanoelectronics, and integrated modeling and test environments.

The scalable applications software effort, called Common HPC Software Support Initiative (CHSSI), is a function of the CTAs. In addition to the essential applications software to be developed in more than 40 projects, CHSSI is expected to produce an enlarged cadre of DoD researchers enabled on scalable parallel machines.

The ten CTA leaders are outstanding practitioners in each area, across the whole range of Army, Navy, and Air Force laboratories. They are chosen by the HPC Modernization Program's Advisory Panel, whose members represent both S&T and DT&E for the Army, Navy, Air Force, Defense Nuclear Agency, and Defense Advanced Research Projects Agency.

The ten CTAs, with leaders identified, are described in the following, and the success stories in this publication are organized by CTAs. The Integrated Modeling and Test Environments (IMT) CTA was formed too recently for IMT-specific success stories to be included in this volume. However, the reader will find a few IMT-related stories in other CTA sections.

### Computational Structural Mechanics (CSM)

*Mr. Kent Kimsey — CTA Leader*
*Army Research Laboratory*
*Aberdeen Proving Ground, MD*

Computational Structural Mechanics is concerned with high-resolution multidimensional modeling of materials and structures subjected to a broad range of loading conditions, including static, dynamic, and impulsive. CSM encompasses a wide range of engineering problems in solid mechanics such as linear elastic stress analysis, material or structural

response to time-dependent loading, large deformations, shock wave propagation, plasticity, frequency response, and nonlinear material behavior. High performance computing for CSM addresses the accurate numerical solution of conservation equations, equations of motion, and constitutive relationships to model simple or complex geometries and material properties, subject to external boundary conditions and loads. CSM is used for basic studies in continuum mechanics, stress analysis for engineering design studies, and predicting structural and material response to impulsive loads. DoD application areas include conventional underwater explosion and ship response, structural acoustics, coupled field problems, space debris, propulsion systems, structural analysis, total weapon simulation, weapon system lethality/survivability, theater missile defense lethality analyses, optimization techniques, and real-time, large-scale soldier- and hardware-in-the-loop ground vehicle dynamic simulation.

**Computational Fluid Dynamics (CFD)**

*Dr. Jay Boris — CTA Leader*
*Naval Research Laboratory*
*Washington, DC*

Computational Fluid Dynamics addresses numerical computation whose goal is accurate solution of the equations describing fluid and gas motion and the complementary use of digital computation in fluid-dynamics testing and experimentation. CFD is used for basic studies of fluid dynamics, for engineering design of complex flow configurations, and for predicting the interactions of chemistry with fluid flow for combustion and propulsion. It is also used to interpret and analyze experimental data and to extrapolate into regimes that are inaccessible or too costly to study. Work in the CFD CTA encompasses all velocity flow regimes and scales of interest to the DoD. Incompressible flows are slow, e.g., governing the dynamics of submarines, slow airplanes, pipe flows, and air circulation. Compressible flows are important at higher speeds, e.g., controlling the behavior of transonic and supersonic planes, missiles, and projectiles.

Fluid dynamics itself displays some very complex physics, such as boundary-layer flows, transition to turbulence, and turbulence dynamics, that require continued scientific research. CFD also must incorporate complex additional physics to deal with many real-world problems. This may entail additional force fields, coupling to surface atomic physics and microphysics, changes of phase, changes of chemical composition, and interactions among multiple phases in heterogeneous flows. Examples of these physical complexities include Direct Simulation Monte Carlo and plasma simulation for atmospheric re-entry, microelectromechanical systems (MEMS), materials processing, and magnetohydrodynamics (MHD) for advanced power systems and weapons effects. CFD has no restrictions on the geometry and includes motion and deformation of solid boundaries defining the flow.

**Computational Chemistry and Materials Science (CCM)**

*Capt. Scott G. Wierschke, USAF — CTA Leader*
*Phillips Laboratory*
*Edwards AFB, CA*

Computational Chemistry and Materials Science includes computational prediction of basic properties of new chemical species and materials that may be difficult or impossible to obtain experimentally. Examples are molecular geometries and energies, spectroscopic constants, intermolecular forces, reaction potential energy surfaces, and mechanical properties. Within DoD, quantum chemistry and molecular dynamics methods are used to design new chemical systems for fuels, lubricants, explosives, rocket propellants, catalysts, and chemical defense agents. Also within DoD, solid-state modeling techniques are used to develop new high-performance materials for electronics, optical computing, advanced sensors, aircraft engines and structures, semiconductor lasers, laser protection systems, advanced rocket engines components, and biomedical applications.

**Computational Electromagnetics and Acoustics (CEA)**

*Dr. Joseph J.S. Shang — CTA Leader*
*Wright Laboratory*
*Wright-Patterson AFB, OH*

Computational Electromagnetics addresses high-resolution multidimensional solutions of Maxwell's equations. DoD applications include calculating the electromagnetic (EM) fields around antenna arrays; the EM signatures of tactical ground, air, sea, and space vehicles; EM performance and design factors for EM gun technology; the EM signature of buried munitions; high-power microwave performance, as well as interdisciplinary applications in magnetohydrodynamics and laser systems.

Computational Acoustics addresses high-resolution multidimensional solutions of acoustic wave equations in solids, fluids, and gases. DoD applications include the modeling of acoustic fields for surveillance and communication, seismic fields for mine detection, and the acoustic shock waves of explosions for antipersonnel weapons.

**Climate/Weather/Ocean Modeling (CWO)**

*Dr. Joseph McCaffrey — CTA Leader*
*Naval Research Laboratory*
*Stennis Space Center, MS*

Climate/Weather/Ocean Modeling is concerned with the accurate numerical simulation of Earth's climate and the simulation and forecast on important space and time scales of oceanic variability (e.g., temperature, salinity, currents, tides, waves, ice motion and concentration, sediment transport, optical clarity) and atmospheric variability (e.g., temperature, winds, pressure, relative humidity, cloud cover, precipitation, storms, aerosols and

trace chemicals, surface fluxes) for both scientific understanding and DoD operational use. Numerical simulations and forecasts are performed from the very top of the atmosphere to the very bottom of the ocean. CWO includes the development of numerical algorithms for assimilating in situ and remotely sensed observations into numerical forecast systems. CWO is used on a daily basis within DoD for safety of flight, search-and-rescue, mission planning, electro-optical propagation, optimal aircraft and ship routing, antisubmarine and undersea warfare, and weapon system design. This CTA provides DoD with high-resolution weather and sea state forecasts; realistic simulations of the dynamic oceanic and atmospheric environment to permit effective mission planning, rehearsal, and training; more effective materiel acquisition; and an improved capability to predict magnetic storm-induced outages of $C^3$, surveillance, and navigation systems.

**Signal/Image Processing (SIP)**

*Dr. Richard Linderman — CTA Leader*
*Rome Laboratory*
*Griffiss AFB, NY*

Signal/Image Processing is concerned with the extraction of useful information from sensor outputs in real time. DoD applications include surveillance, reconnaissance, intelligence, communications, avionics, smart munitions, and electronic warfare. Sensor types include sonar, radar, visible and infrared imagers, and signal intelligence (SIGINT) and navigation assets. Typical signal processing functions include detecting, tracking, classifying, and recognizing targets in the midst of noise and jamming. Image processing functions include the generation of high-resolution low-noise imagery and the compression of imagery for communications and storage. This CTA emphasizes research, evaluation, and test of the latest signal processing concepts directed toward these embedded systems. These processors are usually aboard deployable military systems and hence require ruggedized packaging and minimum size, weight, and power. System affordability is expected to improve by an order of magnitude through the development of scalable codes running on flexible HPC systems. This will allow commercial off-the-shelf HPC-based equipment to replace the traditional, expensive, military-unique "black boxes" that were required to implement high-speed signal/image processing.

**Forces Modeling and Simulation/C4I (FMS)**

*Mr. Robert Wasilausky — CTA Leader*
*Navy Command, Control and Ocean Surveillance Center (NRaD)*
*San Diego, CA*

Forces Modeling and Simulation/C4I addresses the use of command, control, communications, computers, and intelligence (C4I) systems to manage a battle space; the use of large-scale simulations of complex military engagements to facilitate mission rehearsal/training, mission planning, and postmission analysis; the use of collaborative planning to

support real-time decision making; and the use of digital library technology for support of FMS/C4I research and development activities. Across the DoD, the variety of applications is large—with a remarkable diversity of purpose, scope, resolution, emphasis, and time of effect. Common technology threads include object-oriented, distributed, parallel, highly computation and communications intensive, and time-sensitive attributes. Applications exist in design, development, test, evaluation, deployed systems, and training systems.

**Environmental Quality Modeling and Simulation (EQM)**

*Dr. Jeffery P. Holland — CTA Leader*
*Army Engineer Waterways Experimental Station*
*Vicksburg, MS*

Environmental Quality Modeling and Simulation is concerned with the high-resolution, three-dimensional Navier-Stokes modeling of hydrodynamics and contaminant and multiconstituent fate/transport through the aquatic and terrestrial ecosystem and wetland subsystems, their coupled hydrogeologic pathways, and their interconnections with numerous biological species. Within DoD, this technology is used for stewardship and conservation of natural and cultural resources, optimal design and operation of installation restoration, and enhancement alternatives and development of short- and long-term strategies for integrated management to support installation environmental quality. Also of interest to DoD is work in the area of noise evaluation and abatement and water quality models.

**Computational Electronics and Nanoelectronics (CEN)**

*Dr. Barry S. Perlman — CTA Leader*
*Army Research Laboratory*
*Ft. Monmouth, NJ*

Computational Electronics and Nanoelectronics addresses the accurate design and efficient numerical modeling and simulation of complex electronic devices, integrated circuits, and super components. Generally, the goal of research in this area is to lower the cost and/or enable improved performance of DoD electronics through a variety of computer-aided design/computer-aided engineering and predictive modeling and simulation techniques. These include linear and nonlinear analysis; time- and frequency-domain modeling; physics-based transport, diffusion, and tunneling in semiconductors; quantum transport in "designer" electronic materials; electromechanics; and structural analysis of microelectronics. Areas of investigation of interest to DoD include analog/digital high-frequency circuit and device simulation and optimization; modeling and simulation of time/field-dependent quantum transport; nonlinear analysis and particle simulation of fast and slow wave electrodynamic structures; modeling and simulation of microelectromechanical devices and micro-resonators; computational EM/numerical methods for active and passive microwave and millimeter-wave circuits and structures; analysis of coupled nonlinear devices; noise

and stochastic modeling; electronic/photonic interconnect and packaging analysis; neural networks and formal design methods; statistical analysis, design, and synthesis; design-for-test; and fault modeling.

### Integrated Modeling and Test Environments (IMT)

*Dr. Andrew Mark — CTA Leader*
*Army Research Laboratory*
*Aberdeen Proving Ground, MD*

Integrated Modeling and Test Environments addresses the application of integrated modeling and simulation tools and techniques with live tests and hardware-in-the-loop simulations for testing and evaluating DoD weapon components, subsystems, and systems in virtual and composite virtual/real environments. DoD application areas focus on multidisciplinary computational methods and real-time techniques. These include digital scene generation, six degrees-of-freedom trajectory simulations, real-time test-data analysis and display systems for test control and evaluation, and other modeling and simulation integration tools necessary for high-fidelity engineering and closed-loop engagement models (one-on-one and few-on-few) for simulating weapon component subsystems and systems in a virtual operational context.

## ORGANIZATION OF SUCCESS STORIES

This publication consists of abstracts of successful mission results in science, technology, test, and evaluation achieved by DoD scientists and engineers using HPC—primarily at the Major Shared Resource Centers and Distributed Centers of the HPC Modernization Program but including some others as well. The abstracts are organized so that each one appears with the CTA that provides the focus for the research. The abstracts illustrate the role of HPC in basic and applied research, at DoD laboratories and supporting academic and industrial contractors, with results that are significant to both warfighting and civilian purposes. Thus, there is a broad spectrum of results. The difference in objectives across this spectrum must be appreciated to understand the research mission successes reported. To enhance this understanding, individual success stories are given in a standard format:

| | | |
|---|---|---|
| Computer Resource | — | identifies the specific computer used for the research and the DoD or other site that provided it |
| Research Objective | — | identifies the research objective in terms of basic or applied objectives |
| Methodology | — | approach to problems in terms of hardware, algorithm, scalability, scalable efficiency, critical element, etc. |
| Results | — | to research objective and to computational science, if any |
| Significance | — | to basic science, DoD mission, civilian sector |

## LABORATORIES/CENTERS RESPONSIBLE FOR REPORTED RESEARCH

### Army

Army Research Office (ARO), Research Triangle Park, NC
Army Research Laboratory (ARL), Aberdeen Proving Ground, MD; Ft. Monmouth, NJ
Army High Performance Computing Research Center (ARL/AHPCRC), Minneapolis, MN
Army Engineer Waterways Experiment Station (CEWES), Vicksburg, MS
Army Armament Research, Development, and Engineering Command (ARDEC), Picatinny Arsenal, NJ
Army Natick Research, Development, and Engineering Center (NRDEC), Natick, MA
Army Aeroflightdynamics Directorate, Aviation and Troop Command (ATCOM), Moffett Field, CA
Army Dugway Proving Ground, UT

### Navy

Office of Naval Research (ONR), Arlington, VA
Naval Surface Warfare Center (NSWC), Carderock, MD; Bethesda, MD; Chesapeake, VA
Naval Command, Control, and Ocean Surveillance Center, Research and Development Division (NRaD), San Diego, CA
Naval Research Laboratory (NRL), Washington, DC; Stennis Space Center, MS; Monterey, CA
Naval Air Warfare Center, Weapons Division (NAWCWD), China Lake, CA
Naval Air Warfare Center, Aircraft Division (NAWCAD), Warminster, PA
Oceanographer of the Navy, Washington, DC

### Air Force

Air Force Office of Scientific Research (AFOSR), Washington, DC
Wright Laboratory (WL), Wright-Patterson AFB, OH
Phillips Laboratory (PL), Edwards AFB, CA; Hanscom AFB, MA; Kirtland AFB, NM
Rome Laboratory (RL), Griffiss AFB, NY
Air Force Development Test Center (AFDTC), Eglin AFB, FL
Air Force Institute of Technology (AFIT), Dayton, OH

### Defense Nuclear Agency, Alexandria, VA

## MAJOR SHARED RESOURCE CENTERS (MSRCs)

| | |
|---|---|
| Army Research Laboratory (ARL)<br>Aberdeen Proving Ground, MD | SGI Power Challenge Array (96 processors) |
| Aeronautical Systems Center (ASC)<br>Wright-Patterson AFB, OH | Intel Paragon (368 processors) |
| Army Engineer Waterways Experiment Station (CEWES)<br>Vicksburg, MS | Cray C916/1024 (16 processors)<br>Cray Y-MP/8/128 (8 processors) |
| Naval Oceanographic Office (NAVOCEANO)<br>Stennis Space Center, MS | Cray C916/1024 (16 processors)<br>Cray Y-MP/8/128 (8 processors) |

## DISTRIBUTED CENTERS (DCs)

| | |
|---|---|
| Arnold Engineering Development Center (AEDC)<br>Arnold AFB, TN | 2 Convex C4640 (4 processors)<br>Convex C3880 (8 processors)*<br>Convex SPP2000 XA/24 (24 processors)* |
| Air Force Development Test Center (AFDTC)<br>Eglin AFB, FL | Cray T3D (128 processors) |
| Army High Performance Computing Research Center (AHPCRC)<br>Minneapolis, MN | TMC CM-5 (896 processors) |
| Maui High Performance Computing Center (MHPCC)<br>Maui, HI | IBM SP2 (400 processors)<br>IBM SP2 (80 processors) |
| Naval Command, Control and Ocean Surveillance Center (NCCOSC)<br>San Diego, CA | Intel Paragon (336 processors)<br>Convex SPP-1 (32 processors) |
| Naval Research Laboratory (NRL)<br>Washington, DC | TMC CM-5E (256 processors)** |
| Naval Underwater Warfare Center (NUWC)<br>Newport, RI | Cray T3D (64 processors) |
| Rome Laboratory (RL)<br>Griffiss AFB, NY | Intel Paragon (304 processors) |
| Naval Air Warfare Center Aircraft Division (NAWCAD)<br>Patuxent River, MD | TBD |
| Army Tank-Automotive Research, Development, and Engineering Center (TARDEC)<br>Warren, MI | SGI Power Challenge Array (64 R10000 processors) |
| White Sands Missile Range, NM | TMC CM-500 |

*Not yet deployed
**Upgraded to TMC CM-500e

| | |
|---|---|
| Silicon Graphics Incorporated | Convex Technology Center of Hewlett-Packard Company |
| Intel Corporation | Thinking Machines Corporation |
| Cray Research, Inc. | IBM Corporation |

# Success Stories

# Listing

# Success Stories — Listing

## Computational Structural Mechanics (CSM)



## Computational Fluid Dynamics (CFD)

## Computational Chemistry and Materials Science (CCM)

## Computational Electromagnetics and Acoustics (CEA)



## Climate/Weather/Ocean Modeling (CWO)

## Signal/Image Processing (SIP)



## Forces Modeling and Simulations C4I (FMS)

## Environmental Quality Modeling and Simulation (EQM)



## Computational Electronics and Nanoelectronics (CEN)

# Success Stories

# Computational Structural Mechanics

*Computational Structural Mechanics (CSM) addresses high resolution, multidimensional modeling of materials and structures subjected to a broad range of loading conditions including static, dynamic, and impulsive. High performance computing for CSM entails the accurate numerical solution of the conservation equations, equations of motion, and constitutive relationships used to model complex geometries and materials subjected to external boundary conditions and loads.*

*The CSM success stories that follow were chosen to illustrate the wide range of defense applications in CSM. Service-related finite-element applications include, among others, protection of hardened structures, structural integrity to underwater explosions, and structural response to blast loads. Two papers discuss the application of nonlinear mathematical optimization methods for design optimization, and the paper by Costanzo and Camp illustrates the role of transient shock analyses in support of Live Fire trials. The following success stories are prime examples that exploit HPC technology in DoD's RDT&E programs.*

Mr. Kent Kimsey
Army Research Laboratory
Aberdeen Proving Ground, MD
CTA Leader for CSM

# Antipenetration Screen to Protect Hardened Structures

M.D. Adley
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

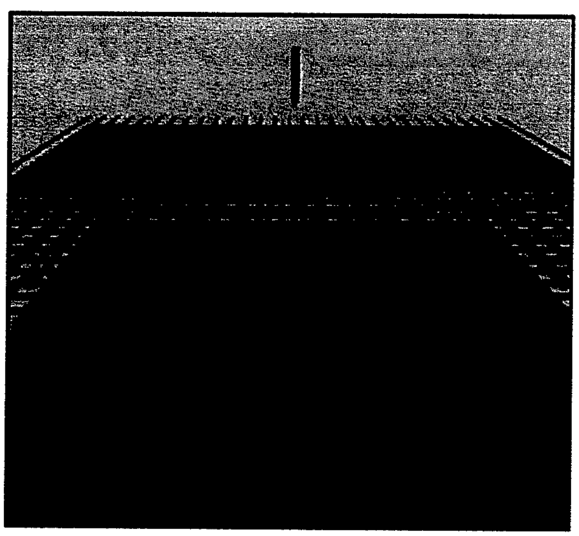
***Computer Resource:*** Cray Y-MP [CEWES MSRC]

***Research Objective:*** To evaluate the structural response of hard-target penetrating weapons impacting hardened military structures.

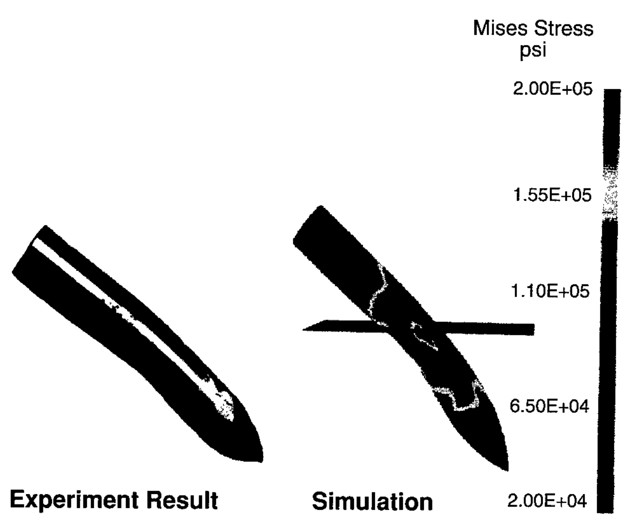
***Methodology:*** A new computational methodology developed at CEWES for simulating projectile structural response to hard-target impact has resulted in a simply coupled penetration trajectory/structural dynamics code. The code was developed by linking the CEWES rigid-body penetration trajectory code PENCURV with the general-purpose finite code ABAQUS. The resulting code can simulate very general impact problems, including those that involve three-dimensional impact conditions and complex geologic/structural targets. The projectile is modeled as a 3-D shell element structure accounting for material and geometric nonlinearities, which effect the response of the projectile. The target is modeled by the penetration trajectory code, which uses empirically based forcing functions in conjunction with layer interface/free-surface effect algorithms to simulate the penetration resistance of the target.

***Results:*** The aforementioned code was used to design a protective structure concept consisting of a yaw-inducing screen and a concrete burster-slab for defeating penetrating weapons. Parametric calculations were conducted on the Cray Y-MP to ensure that a sufficient level of damage was sustained by the projectile.

***Significance:*** The coupled code has been used to develop several protective structure concepts and to determine the failure mechanisms for penetrating weapons as a function of impact conditions and structure design. Recent analyses have determined the failure mode of a general-purpose bomb impacting a NATO-designed articulated burster slab and evaluated the efficacy of two penetrating weapons for the Defense Nuclear Agency.



*Artist's rendering of yaw-inducing bar screen*




*Projectile impacting concrete burster slab with high angle of attack*

# Optimal Warhead Design

E.L. Baker
*Army Armament RD&E Center, Picatinny Arsenal, NJ*

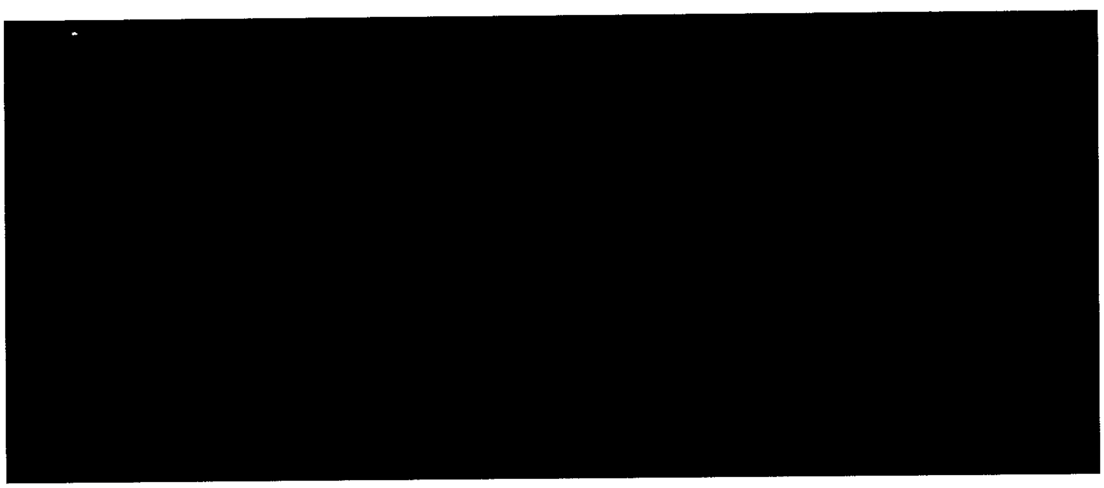
***Computer Resource:*** SGI Power Challenge Array [ARL MSRC]

Research Objective: The Energetics and Warheads Division at the Army Armament RD&E Center (ARDEC) is involved in the development of antiarmor warheads. Modern, explosively formed projectile (EFP) warheads employ an explosive charge to project and form a metal liner to produce a high-velocity penetrator. The ARDEC Target Defeat Program is developing optimal warhead design technology that would provide increased warhead lethality with reduced weight and cost.

***Methodology:*** Nonlinear optimization is being investigated to replace labor-intensive manual warhead design iterations based on finite-element models. Numerical optimization design iterations replace manual design iterations with an optimization algorithm that iteratively evaluates finite-element warhead models searching for the optimal design. The computer program being used to do the optimization is NLQPEB, a variable metric sequential quadratic programming routine under development at ARDEC.

***Results:*** The problem illustrated is the optimal design of an EFP. The NLQPEB optimization routine was coupled to DYNA2D, a Lagrangian finite-element code. Nonlinear optimization was used to redesign optimally the warhead liner of a generic EFP. The optimization required about 10 hours on a Silicon Graphics Power Challenge computer workstation. The optimized EFP is 15% longer than the original EFP.

***Significance:*** The application of state-of-the-art optimization technology not only dramatically reduces warhead design development time and cost, but also allows the development of fully optimized penetrator shapes producing up to 15% lethality increases not previously possible using conventional design methodology. An anticipated CHSSI software project will put this technology on highly scalable computer platforms. This should further increase warheads lethality as well as design capabilities for both military and commercial applications.



*Nonlinear optimization of warhead design: original (left) and optimized (right) explosively formed penetrator based on finite-element analyses*

# Stresses in Ship Hull

R.S.-C. Cheng, G.C. Everstine, and E.G. Fishlowitz
*Naval Surface Warfare Center, Bethesda, MD*

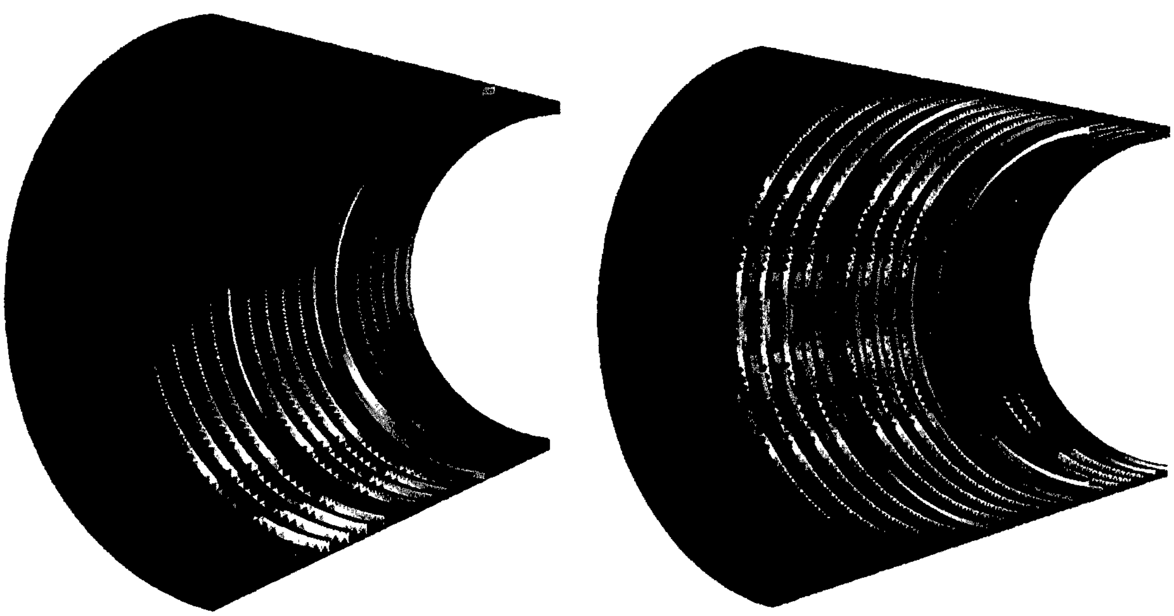
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** The Navy has a new acoustic test facility in which a scale-model submarine hull is submerged in a deep lake. During testing, the model is subjected to a variety of unusual loadings because of the various rotated orientations used and the presence of ballast trays. A critical problem was to establish in advance the integrity and safety of the hull when subjected to the anticipated loads due to the ballast trays. The objective of the study was to perform a stress analysis of the stiffened hull to assess the hull strength.

***Methodology:*** A detailed finite-element prediction model was prepared and run using the general-purpose structural analysis software CSA/NASTRAN. Because great detail was needed for the stress predictions in the hull plating and stiffener webs and flanges, the resulting model required over 100,000 degrees of freedom, necessitating the use of high performance computers.

***Results:*** The analysis indicated that the stresses were at an acceptable level even when the hull was rolled (rotated) up to 90 degrees. The figures below show typical stress contour plots of maximum principal stress for two orientations.

***Significance:*** The findings allow acoustic testing of the scale-model hull to proceed with confidence that there would be no damage to the test model. This testing is critical to ensure the quiet operation of U.S. submarines.



*Major principal stresses in hull model subjected to ballast tray loads*

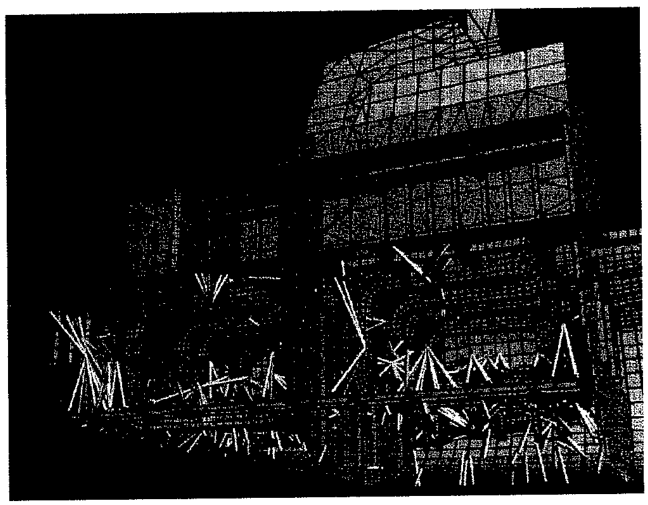
# Transient Shock Response of a Composite Minehunter

F.A. Costanzo and G.H. Camp IV
*Naval Surface Warfare Center, Chesapeake, VA*

***Computer Resource:*** Cray C916 [CEWES MSRC]

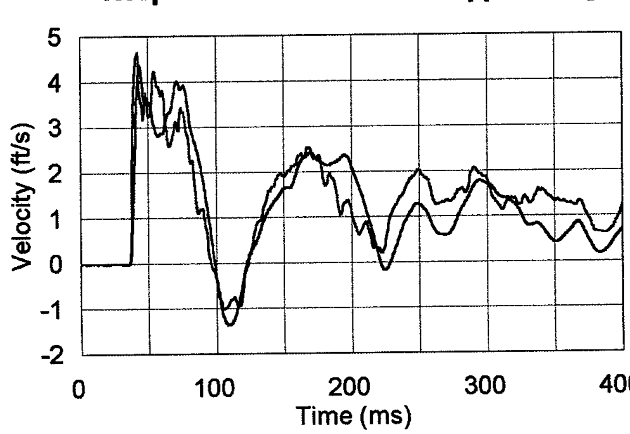
***Research Objective:*** To evaluate structural integrity of coastal minehunters that are subjected to a series of underwater explosions of increasing severity.

***Methodology:*** A new class of coastal minehunter constructed from composite materials was subjected to a series of underwater explosion shock trials of increasing intensity. Transient shock analyses were performed to assess the performance of the ship's complex structural configurations throughout the course of these Live Fire trials. These computations were compared with experimental results on-site, and modifications to the dynamic loading functions were made in real time for subsequent tests. The necessary level of detail required the development in CSA/NASTRAN of a finite-element model representing two main equipment rooms with a combined size of 200,000 degrees of freedom. Quick turnaround of analysis results on the CEWES Cray C916 was paramount to the overall success of the trials in meeting both the technical and programmatic requirements.



*Cutaway view of finite-element model of equipment rooms*

***Results:*** Pre-trials predictions in the way of time history response plots and animation videos were generated prior to the commencement of the Live Fire trials. Between tests, modifications were made to both the model and the dynamic loading functions using the measured data from the previous trials, and revised projections for the next trials level were developed. Assessments of these analyses resulted in the formation of a Navy position and recommendation for the safe continuation of the trials.




*Computed results vs Live Fire measurement*

***Significance:*** The Navy views this work as a significant success from a number of viewpoints. As a result of rapid turnarounds of the high performance computer predictions, improved projections to the next shock level based on a combination of pre-trials analyses, shock test data, and physical inspections could be made. This valuable on-site product directly supported the Navy in making timely and critical decisions of whether to proceed to the next level or to terminate the trials. In addition, the Navy has gained immense insight into the shock response behavior of a complex composite ship structure subjected to underwater explosion loadings and has learned more efficient methodologies for solving this type of problem.

# Glass Particle Velocities from Windows Subjected to Blast

S. Garner, J. Watt, and R.L. Hall
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

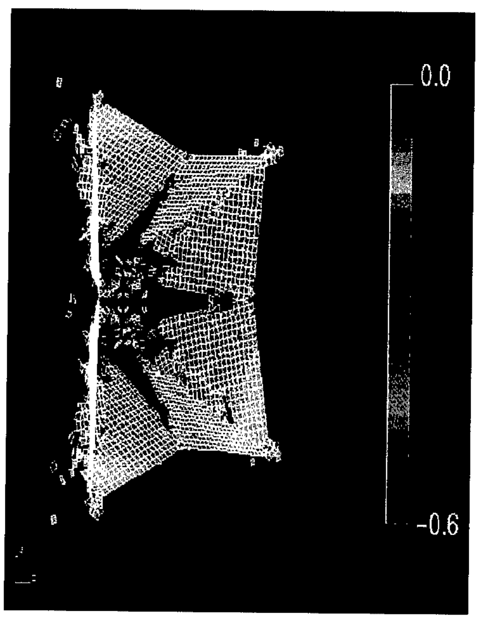
***Computer Resource:*** Cray C916 and Cray Y-MP [CEWES MSRC]

***Research Objective:*** To predict the velocity of glass particles from windows subjected to an explosive charge in order to establish design guidelines for building retrofit techniques for abating injury of the building occupants.

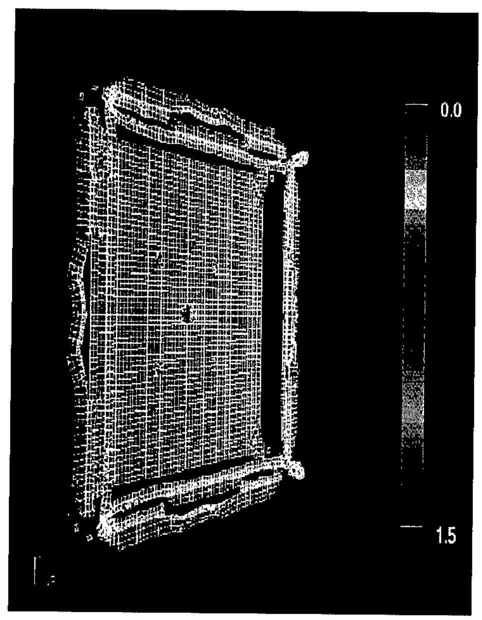
***Methodology:*** The finite-element program, DYNA3D, was used to model single- and double-glazed windows of three sizes and varying thicknesses subjected to pressure loadings from charge weights from 50 to 100 lb at standoff distances of 50 to 500 ft. Analyses predicted previously observed test failure mechanisms and predicted glass fragment velocities that were somewhat conservative when compared with test results. After verification of the analyses results, additional analyses were run to supplement and expand available test data. The resulting data were then used to develop a predictive tool based on load impulse and pressure, window size, and glass strength and thickness.

***Results:*** From a fit to the analyses results, equations have been developed for predicting the velocity of glass particles based on window size, glass thickness and strength, and loading pressure and impulse. Predictions based on these equations correspond well with experimental results and can be extrapolated to other loadings and window characteristics. The figures below demonstrate two different failure mechanisms of unretrofitted single-pane glass windows.

***Significance:*** The extent of the threat to building occupants of glass fragments resulting from terrorist bombings can be established. Retrofit techniques to diminish this risk in existing buildings have been investigated.




*Bending failure of single-pane glass window under blast loading*




*Shear failure of single-pane glass window under blast loading*

# Rigid Pavement Response Modeling

M.I. Hammons
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

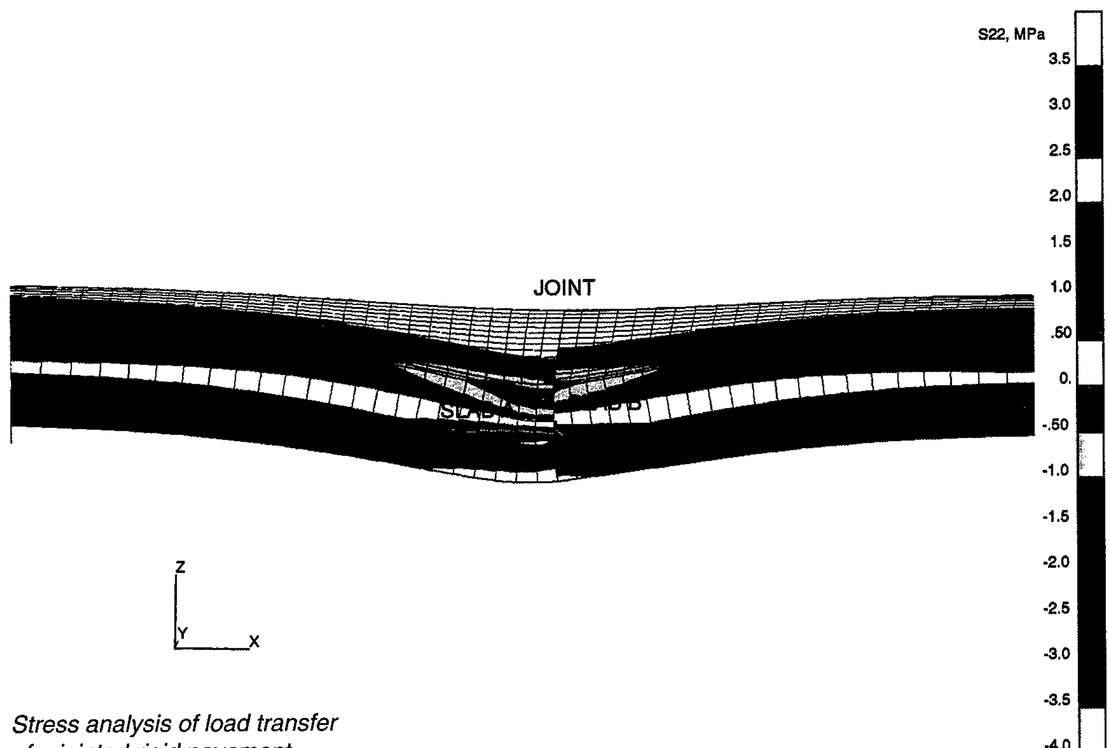
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To develop a three-dimensional response model of the rigid pavement, slab-joint-foundation system that will be used to improve rigid pavement design criteria by increasing pavement life while reducing life-cycle costs.

***Methodology:*** Comprehensive 3-D modeling of the rigid pavement system provides a more fundamental understanding of certain aspects of rigid pavement response that can be incorporated into the design process. Adequate representation of this system requires a 3-D analytical approach. A general, 3-D, finite-element model was developed that included the joint and interfaces between the slab and base layer. The model features over 50,000 nodes. Solid sections were modeled with 27-node, second-order Lagrangian, isoparametric, hexahedral elements. Load transfer at joints was modeled using general, 3-D, nonlinear spring elements along the vertical faces of the joint. The boundary between the slab panels and the sub-base was modeled using 9-node interface elements. These elements are formulated to model contact and friction over part or all of the areas of the contact surfaces.

***Results:*** Certain long-standing assumptions concerning the response of rigid pavements have been proven to be inconsistent. The classical rigid pavement response model is Westergaard's theory, which models a slab-on-grade as a thin plate supported by a bed of springs. Results from the 3-D finite-element analysis have shown that Westergaard's theory overestimates bending stresses near the boundaries of the slab. The impact of these inconsistencies on pavement behavior and performance is currently being assessed.

***Significance:*** The findings of this research will enable DoD to design, construct, and maintain pavement facilities well into the 21st century. The magnitude of the existing DoD pavement investment ($85 billion in existing facilities plus $500 million per year in construction and maintenance) dictates a need for this design and analysis capability.




*Stress analysis of load transfer of a jointed rigid pavement*

# Modeling Granular Deformation

D.A. Horner and J.F. Peters
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

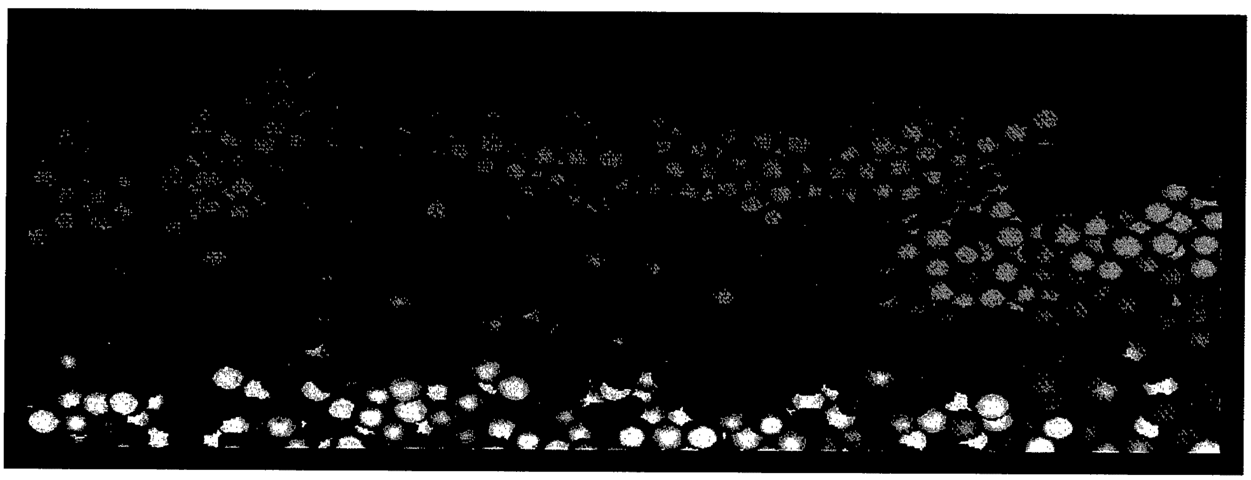
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To develop a theory for mechanics of granular media for complex soil deformations that occur in vehicle-soil interactions, for example, military engineering vehicle plowing operations.

***Methodology:*** We have developed a smoothed approximation to a discrete element model for numerical approximation of granular flow. This discrete element model is an alternative to a classical continuum mechanics approach for describing soil response but is not controlled by compatibility relationships that traditionally limit analyses to small strain. The particle model treats the soil as a collection of individual unconnected particles whose motions are controlled by Newton's law of momentum conservation. The number of particles required by discrete-element models to represent soil in most practical problems exceeds $10^9$. The intent of the smoothed equations is to model discontinuous flowlike deformations of the soil using a relatively small number of computational particles ($<10^6$). The project requires high performance computing resources because the development of the constitutive relationships for the smoothed model requires "measurements" from a numerical laboratory that can model large particle systems. Also, the tendency for localized deformations in the smoothed model requires high resolution simulations.

***Results:*** Various boundary value problems have been simulated. The simulations involved many phases of granular materials. Trapdoor experiments displayed solids, fluids, and gases. Penetration and pullout experiments displayed solid behavior and contained fluid flow. Plowing experiments displayed solid behavior and fluidity under unconfined flow. Laboratory tests have been simulated to obtain constitutive properties from statically homogeneous specimens.

***Significance:*** The data obtained from the particle simulations contribute directly to a numerical analysis procedure for deformation of granular materials. This more general computational procedure for large discontinuous deformation problems will benefit the Army's ability to model vehicle-soil interaction problems such as the plowing performance of military engineering vehicles. Benefits to the Army derived from this research include a more accurate understanding of terrain influence on off-road vehicle mobility, better design traction elements, and less dependence on full-scale testing to develop designs of next generation military vehicles.



*Soil/tire interaction simulation*

# Optimum Design of an Actively Controlled Composite Wing Structure

N.S. Khot and D.E. Veley
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

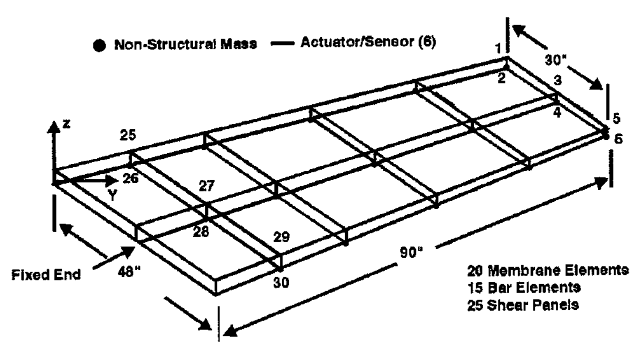
***Computer Resource:*** Cray C916 and Cray Y-MP [CEWES MSRC]

***Research Objective:*** To develop a reliable design procedure for aircraft structures considering simultaneously different disciplines such as structures, robust controls, aerodynamics, and materials.

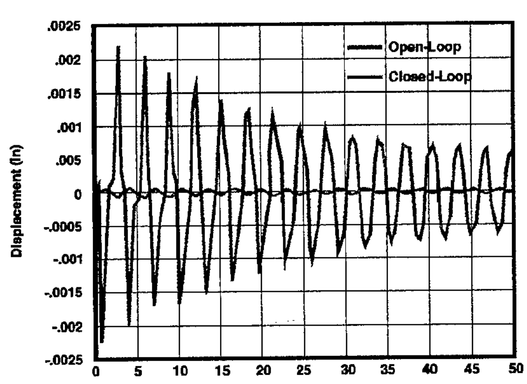
***Methodology:*** The design procedure is formulated as a nonlinear mathematical optimization problem. The objective function to be minimized is the weight of the structure. The constraints are imposed on the response quantities such as frequency distribution, closed-loop damping, closed-loop response singular values, the robustness parameters, the time required to suppress the oscillations, flutter velocity, and the upper and lower bounds of the design variables. The design variables are the cross-sectional areas of the members, thicknesses and fiber orientation of the finite elements, weighting parameters in the control design, and bounds on the control forces. This highly nonlinear problem is solved in an iterative fashion by using both gradient and nongradient-based design algorithms.

***Results:*** This approach was used to design a composite wing structure. The top figure shows the finite-element model used for this investigation. The membrane elements of the top and bottom skins are composite elements with fiber orientations of [0/90/45]. The lower left figure shows the transient response (time history of the displacement of the tip) of the open-loop (uncontrolled) and closed-loop (controlled) system to the external disturbance for the optimized design. The lower right figure shows that the frequency response for the closed-loop system is significantly below that of the open-loop system indicating the robustness of the design.

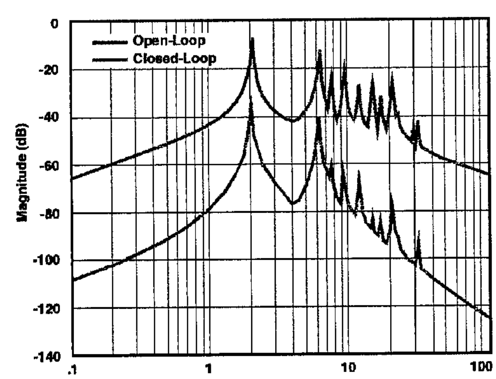
***Significance:*** This design approach would reduce the weight of the structure, enhance the robustness, improve rapid maneuver capability, and increase the payload and range of a typical fighter mission.




*Finite-element model of composite wing structure*




*Transient response*




*Frequency response*

# Conventional Weapon Detonation Inside a Hardened Structure

P.P. Papados and J.T. Baylot
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

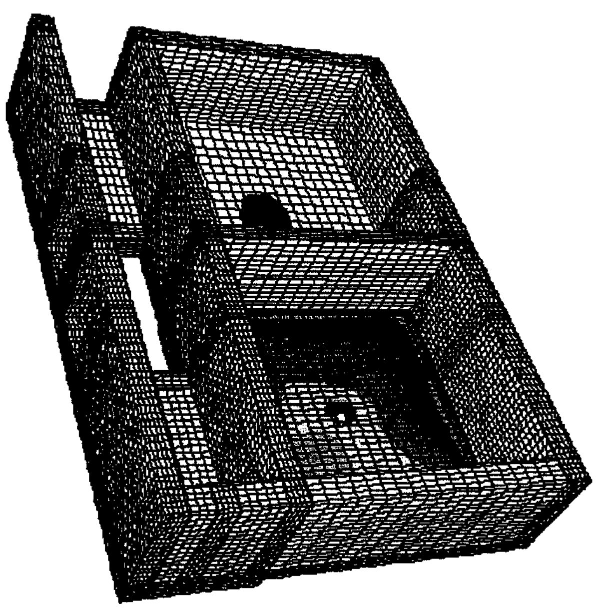
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To investigate damage and failure mechanisms of hardened reinforced concrete (RC) structures subjected to an internal detonation of a conventional weapon.

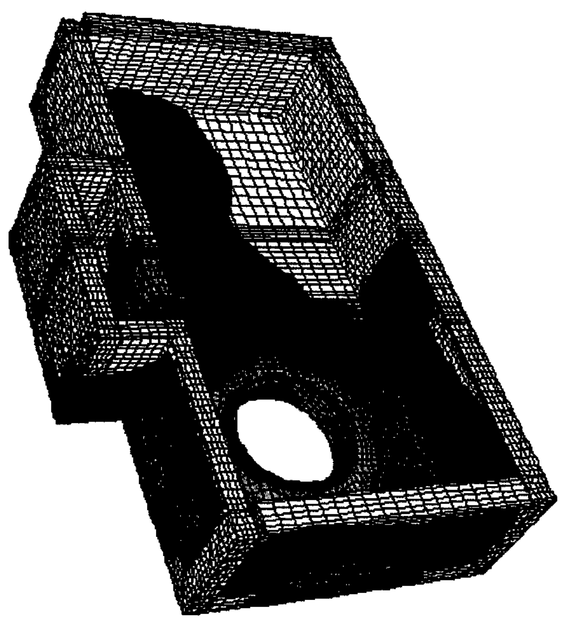
***Methodology:*** The development of precision guided munitions (PGM) has presented new and complex problems in the area of effective design of survivable hardened structures and accurate vulnerability analysis of targeted structures. Accuracies of the PGM often result in weapon detonation inside the structures creating blast pressures and other loads associated with kinetic energies of weapon casing fragments. A finite-element (FE) analysis was carried out to investigate the response of the structure. DYNA3D, a nonlinear, explicit, three-dimensional FE code for solid and structural mechanics was used to carry out the analysis. The model, consisting of approximately 500,000 degrees of freedom, simulated a portion of the overall structure and surrounding soil. The concrete matrix and the reinforcing bars are explicitly modeled with 144,257 solid and 168,438 truss elements, respectively. Pressure-time histories derived from first-principle calculations were used to assign the induced loads onto 17,858 element surfaces. Nonlinear constitutive models were used to simulate the material properties of concrete and the reinforcing steel. The FE analysis was carried out to 60 ms.

***Results:*** The numerical results provide very good correlation with the experimental data and a clearer quantitative understanding of damage and failure mechanisms in hardened structures.

***Significance:*** Estimates of damage inside such structures make it possible to provide accurately bomb damage assessment for hardened targets. These estimates also provide a capability to design compartmentalized structures optimizing wall thickness and, thus, construction cost.



*Finite-element response of concrete hardened structure showing downstairs rooms*



*Finite-element response of concrete hardened structure showing upstairs rooms*

# What If a Plane Crashes into a Chemical Agent Storage Yard?

G. Randers-Pehrson
*Army Research Laboratory, Aberdeen Proving Ground, MD*

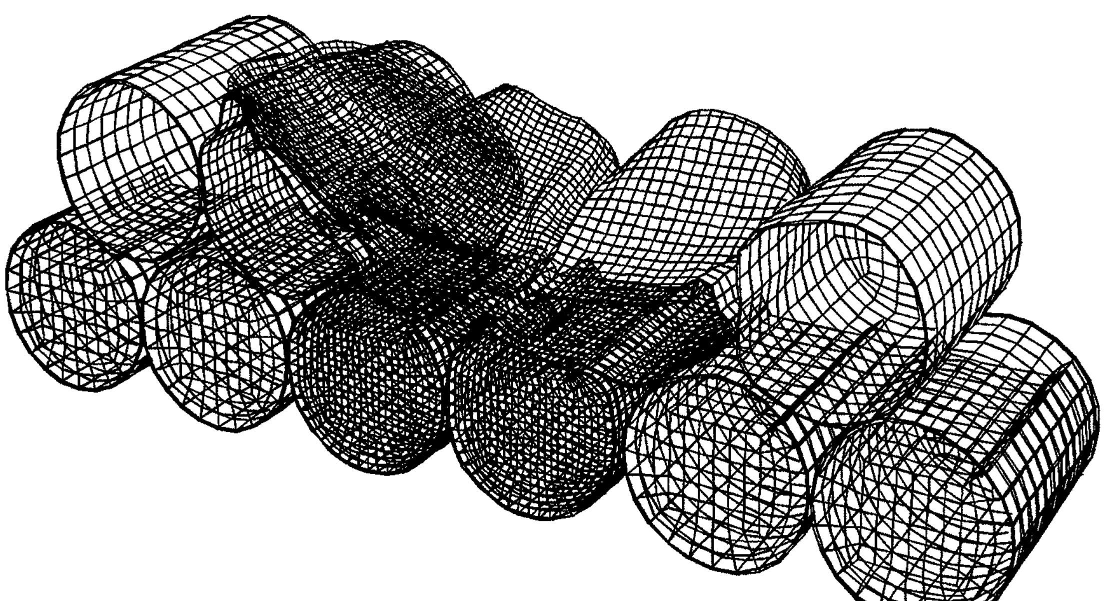
***Computer Resource:*** SGI Power Challenge Array [ARL MSRC]

***Research Objective:*** To determine the response of a stack of one-ton containers of chemical agent (mustard) to impact by an airplane and estimate the effectiveness of a measure for reducing the risk to the surrounding population.

***Methodology:*** This parameter study involved multiple, single-CPU runs with the DYNA3D finite-element code, using 4-node shell and 8-node solid elements. Each problem involved approximately 50,000 finite elements and required 24 to 48 hours of CPU time. The Power Challenge Array ran four to eight problems at a time, with different impact conditions. A graphics postprocessor running on local SGI workstations stored thousands of individual frames for videotape in the efficient new portable network graphics (PNG) format. ARL's Abekas framebuffer equipment made the videotapes, which were essential in visualizing and presenting the results.

***Results:*** The study indicated that this risk-reduction measure is effective in significantly reducing the probability of release of chemical agent outside the storage area in the event of a plane crash into the storage yard.

***Significance:*** This study improves public safety and provides data for emergency planning by the post commander and local government agencies. The results of this study have been used in a recent risk assessment of the storage yard at Aberdeen Proving Ground.



*Result of DYNA3D simulation of a crash at 30 degrees elevation. The risk-reducing empty containers placed on top of the stack are severely damaged, but the full ones below are only slightly dented. The plane is show in green, the tanks in blue, and the chemical agent in brown.*

# Unsteady Aerodynamics for Aeroelastic Analysis Applications

D.M. Schuster
*Lockheed Martin Engineering and Science Services, Hampton, VA*
L.J. Huttsell
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

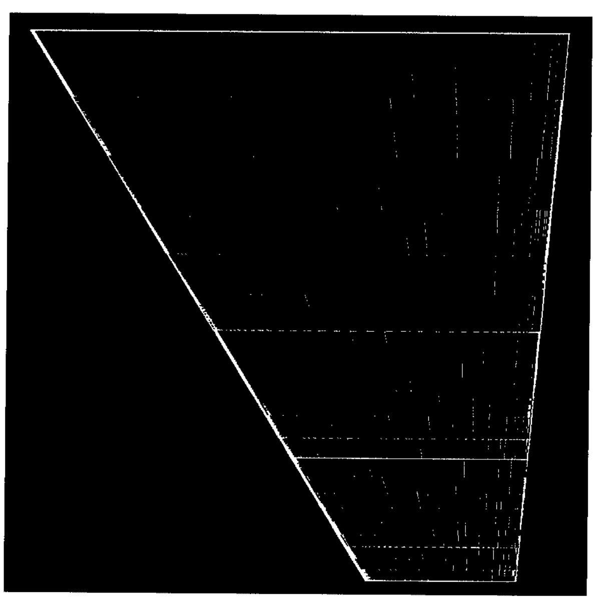
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC] and Cray Y-MP [CEWES MSRC]

***Research Objective:*** Accurate, efficient, unsteady aerodynamic methods are required to perform aeroelastic and multidisciplinary analyses of modern flight vehicles. Wing flutter, analysis of maneuvering aircraft, and aeroservoelasticity all require that unsteady aerodynamics be effectively modeled, often at extreme flight conditions. This research focuses on validating an aeroelastic analysis code, known as ENS3DAE, for unsteady aerodynamic simulations.

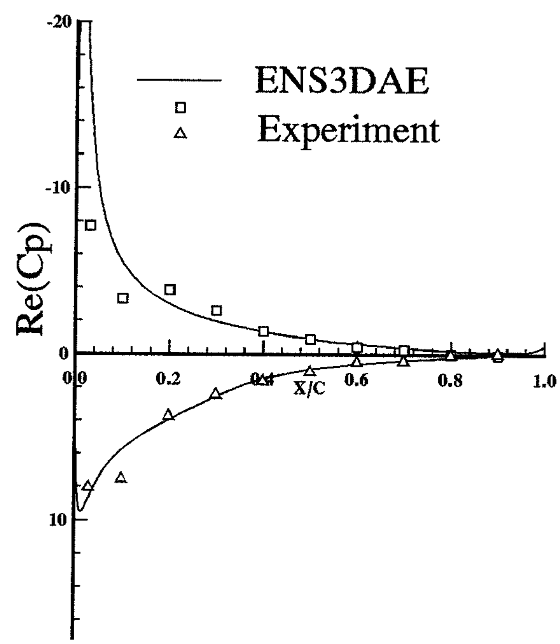
***Methodology:*** ENS3DAE solves the three-dimensional Euler/Navier-Stokes equations in the time domain so that unsteady aerodynamic loads can be simulated on structurally flexible aircraft. The present effort computes the unsteady pressure distribution on the F-5 fighter wing as it is oscillated in pitch. These calculations are compared with available experimental data.

***Results:*** The left-hand figure shows a planform view of the F-5 wing grid used in this analysis; this model consists of 328,125 grid points. The right-hand figure presents the inviscid, unsteady pressure distribution computed by ENS3DAE at M = 0.8, compared with experimental data at 87.5% of the wing semispan. The mean angle of attack for this analysis is 0°, and the pitch amplitude is 0.11° at a frequency of 40 Hz. This plot represents the component of the pressure distribution that is in phase with the wing motion. Similar results are obtained for the out-of-phase pressure.

***Significance:*** Development of accurate unsteady aerodynamic analysis methods allows the aeroelastic performance of aircraft to be simulated, thus allowing costly wind tunnel and flight test experiments to be reserved for cases that cannot be analyzed using theoretical methods.



*Planform view of F-5 wing surface grid*




*F-5 unsteady surface pressure coefficient at M = 0.8, 87.5% span*

# Shipboard Shock-Resistance Evaluation of Advanced Vertical Launch Antisubmarine Rocket

R.C. Shaw

*Naval Command, Control and Ocean Surveillance Center, San Diego, CA*

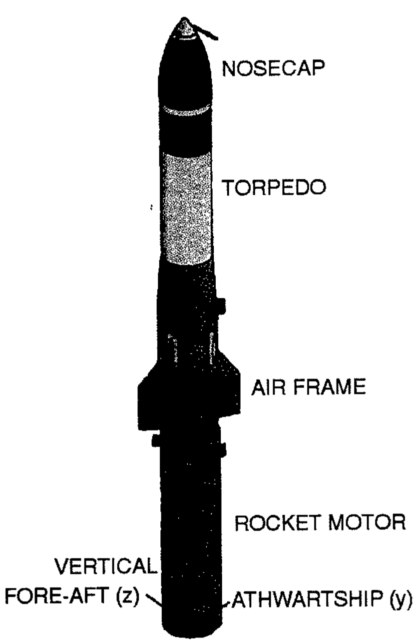
***Computer Resource:*** Convex SPP-1 [NCCOSC DC]

***Research Objective:*** To determine analytically the survivability of the proposed vertical launch antisubmarine (VLA) rocket, configured with an advanced MK 46 torpedo, when subjected to the shipboard shock caused by a near-miss underwater explosion.

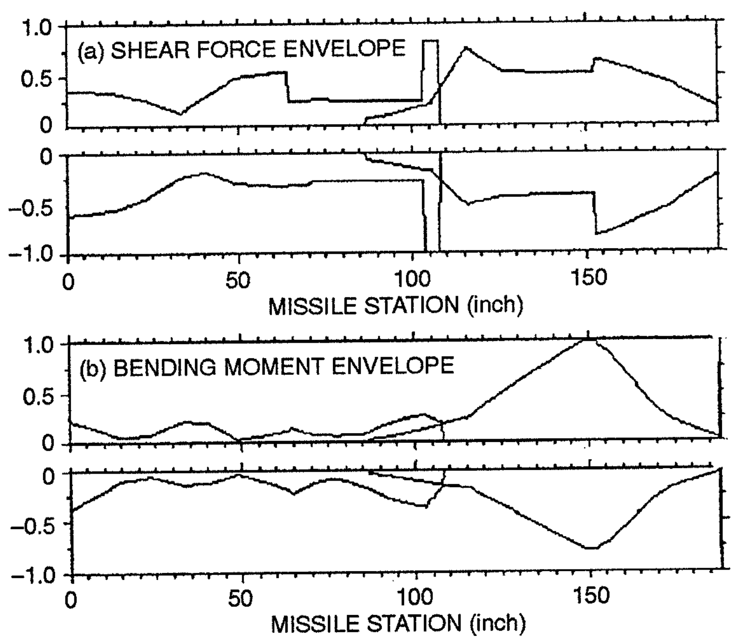
***Methodology:*** The large-mass method, in conjunction with the ABAQUS finite-element, modal dynamic analysis technique, was used to enforce the known acceleration time histories at the missile-canister interface points to excite the VLA missile finite-element model (FEM) so that the response motion at other locations (as well as the internal and external loads of the missile) could be determined. The acceleration histories enforced at the advanced MK 46 VLA missile FEM were the recording data taken at the base and lateral support points of an instrumented VLA missile configured with an original MK 46 torpedo during shock trials aboard the USS *Mobile Bay* (CG 53). The predicted peak response loads were compared with VLA missile allowable loads to determine margins of safety. The acceleration responses of various missile components were used to compute shock response spectra (SRS), which were compared with the missile design requirement SRS curves to detect excessive motion.

***Results:*** The acceleration and response loads of the advanced MK 46 VLA missile, when subjected to CG 53 shipboard shock, were computed with ABAQUS on a minisupercomputer. The envelopes of maximum and minimum responses were derived and plotted as shown below.

***Significance:*** The proposed advanced MK 46 torpedo VLA was determined by the analysis to be questionable in its ability to survive MIL-S-901D Grade A requirements. Grade A items must withstand shipboard shock without an unacceptable effect upon performance and without creating a hazard. However, the analysis also showed that the missile would be capable of MIL-S-901D Grade B requirements that an item must withstand shipboard shock without creating a hazard to personnel or to Grade A equipment.




*Advanced MK 46 torpedo VLA in ship's coordinate system*




*Normalized response load envelopes of advanced MK 46 VLA*

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**Rigid Pavement Response Modeling**

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**Optimum Design of an Actively Controlled Composite Wing Structure**

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N.S. Khot, "Integrated Structural Design and Active Vibration Control," presented at 35th SDM Conference, Hilton Head SC, 18-21 April 1994.

**Conventional Weapon Detonation Inside a Hardened Structure**

J.T. Baylot, P.P. Papados, R.H. Sues, and R.L. Holmes, "Effects of Fragments on Structural Loadings from Conventional Weapons Detonations—Part I," *Proceedings of the 65th Shock and Vibration Symposium*, San Diego, CA, 1994.

P.P. Papados, J.T. Baylot, and R.L. Holmes, "Effects of Fragments on Structural Loadings from Conventional Weapons Detonations—Part II," *Proceedings of the 65th Shock and Vibration Symposium*, San Diego, CA, 1994.

**Shipboard Shock-Resistance Evaluation of Advanced Vertical Launch Antisubmarine Rocket**

"Shipboard Shock Response Analysis of Advanced Vertical Launch Antisubmarine Rocket (VLA)," *Proceedings, The 66th Shock and Vibration Symposium*, Biloxi, MS, 30 October – 3 November 1995. (The symposium was sponsored by U.S. Army Engineer Waterways Experiment Station, and the paper was to be published in the Vol. 3 of the Conference Proceedings by Shock and Vibration Information Analysis Center (SAVIAC), 2231 Crystal Drive, Suite 711, Arlington, VA 22202.)

# Computational Fluid Dynamics

*Computational Fluid Dynamics is the accurate numerical solution of the equations describing fluid and gas motion. CFD, which encompasses nearly half of DoD HPC use, is applied to engineering design of DoD vehicles, facilities, and propulsion systems as well as for fundamental studies of fluid dynamics and turbulence. The 35 CFD success stories that follow illustrate both Grand Challenge science and state-of-the-art engineering by some of DoD's top laboratories, academic partners, and industrial contractors. The first 16 stories show applications of several different generic approaches to "realistic CFD in very complex geometry." This topic is the first of three major thrusts in the Computational Fluid Dynamics technology area of the DoD CHSSI software development program. The next 7 stories describe successes in CFD with complex physics. The final 12 contributions relate success stories of a more fundamental fluid dynamic nature where our understanding of complex fluid flow has been enhanced by the world-class facilities made available through the DoD HPC Modernization Program.*

*Each of the three sections begins with a success story that is being highlighted because of its particularly high impact. The highlighted complex geometry problem is a joint service S&T, DT&E, and academic effort to develop complex modeling tools and techniques to predict deployment of paratroopers from large transport aircraft (see pages 40-41). The highlighted complex physics CFD problem (page 54) is a joint service S&T, DT&E effort to design, test, and license an open-air detonation (OD) facility that promises real savings of more than $1 billion in the removal/destruction of obsolete munitions stored in DoD sites. There are more than half a million tons to be disposed of, and open-air detonation will reduce the cost to reprocess these often-unstable, obsolete munitions by more than a factor of 3. In situ explosion (OD) appears to be practical for less than $1000 per ton. The basic science fluid dynamics highlight involves a breakthrough made possible entirely by Grand Challenge-level HPC (page 63). Magnetic flux tubes have previously been thought to be incapable of passing through each other on the basis of ideal magnetohydrodynamics (MHD). New high-resolution numerical simulations approaching the high Reynolds number limit show that real flux tubes can in fact "tunnel" through each other. This new physical understanding replaces what has been taught for decades in MHD and plasma courses.*

Dr. Jay P. Boris
Naval Research Laboratory
Washington, DC
CTA Leader for CFD

# C-17 Paratrooper Operation

Capt. M.J. Aftosmis, U.S. Air Force
*Wright Laboratory, Wright-Patterson Air Force Base, OH, and NASA Ames, Moffett Field, CA*
H.T. Emsley and J.M. Manter
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

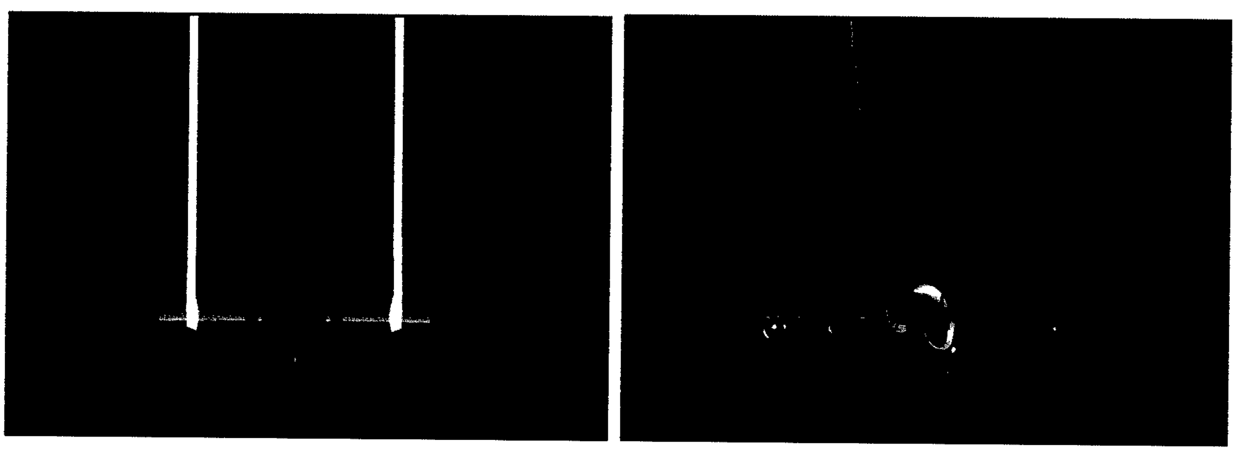
***Computer Resource:*** Cray C916 [CEWES MSRC and NASA Ames, Moffett Field, CA]

***Research Objective:*** To develop an improved understanding of the aerodynamic flowfield encountered by Army paratroopers exiting Air Force transport aircraft. This simulation was requested by a joint Army/-Air Force Executive Independent Review Team (EIRT) tasked with the development of a C-17 configuration satisfying Army requirements for mass paratrooper exits.

***Methodology:*** Inviscid simulations of both the C-141 and C-17 aircraft were accomplished using two unstructured grid codes. The code Cobalt, developed at Wright Laboratory, was used to model the C-141 flowfield. A second code, currently under development in a joint venture between Wright Laboratory and NASA Ames, was used to model the C-17. The second code solves the Euler equations on adaptively refined Cartesian grids and includes the work of Professor M. Berger, which is sponsored by the Air Force Office of Scientific Research.

***Results:*** CFD flowfield simulations were used by the EIRT team to gain insight into the salient features of the C-17 and C-141 flowfields. The team subsequently directed water- and wind-tunnel tests based on a "design of experiments" matrix to determine the configuration that would satisfy Army requirements. The final configuration was confirmed in April 1995, when more than 300 jumpers, spanning 3 sorties, safely exited a C-17 aircraft at the Army's Yuma Proving Ground, Arizona.

***Significance:*** The exercise demonstrated that CFD simulations of complicated USAF configurations can be accomplished with the necessary speed and accuracy to impact positively ongoing developmental ground and flight tests. Research scientists today, starting with a suitable mathematical description of an aircraft surface, can use automated unstructured gridding techniques to perform Euler flowfield simulations in a few days.



*(C-141)* *(C-17)*

*Streamlines behind aircraft at typical speed and configuration for paratrooper exit*

# Three-Dimensional Simulation of Round Parachutes

K. Stein
*Natick Research, Development, and Engineering Center, Natick, MA*
A.A. Johnson and T. Tezduyar
*ARL/Army High Performance Computing Research Center, Minneapolis, MN*

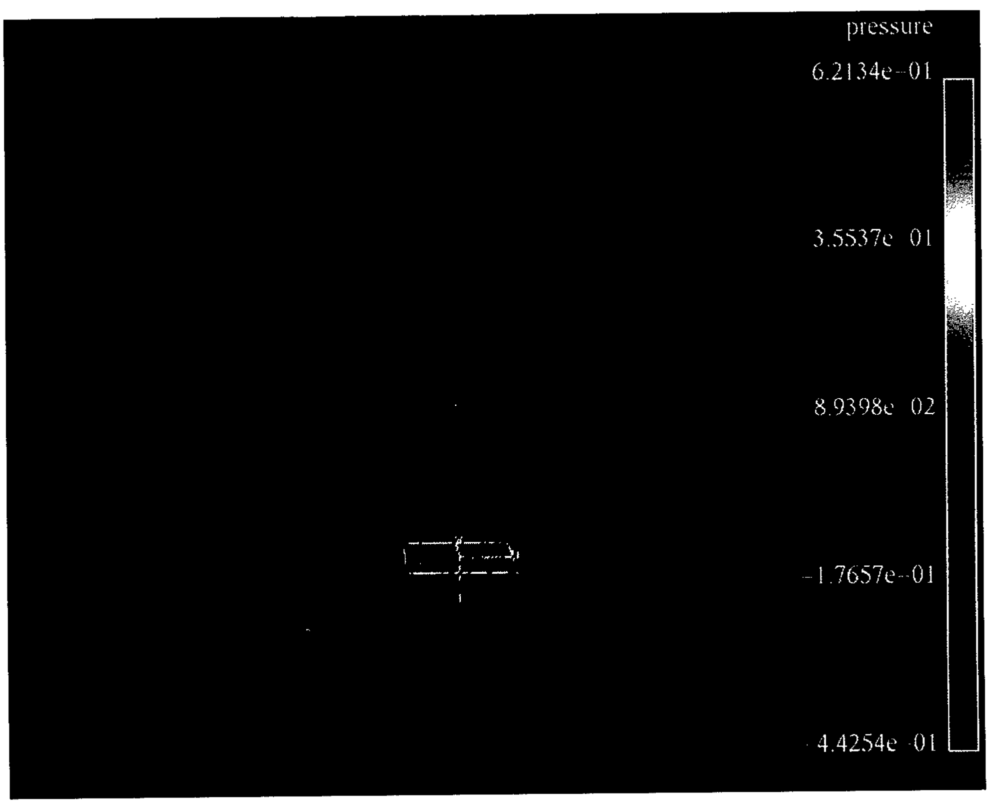
***Computer Resource:*** TMC CM-5 [AHPCRC DC]

***Research Objective:*** To establish numerical modeling methods for parachute design and development. The techniques developed must be applicable to complicated parachute geometries and must be suited for deforming spatial domains in parachute-opening studies.

***Methodology:*** The three-dimensional (3-D) Navier-Stokes equations for incompressible flow are discretized using a stabilized semi-discrete finite-element formulation and an unstructured tetrahedral mesh. The resulting coupled nonlinear equations are solved by an iterative strategy.

***Results:*** These techniques are being used in the simulation of the 3-D flow field about a conventional round parachute. The simulations depicted are for a calculation at a Reynolds number of 1 million based on the projected diameter of the parachute.

***Significance:*** Parachutes and airdrop systems have traditionally been developed by time-consuming and costly full-scale testing. The capability to use parallel computers to model and develop parachutes and airdrop systems will greatly reduce the time and cost of full-scale testing and assist in the optimization of new capabilities. The coupling of such models with structural dynamics models for the parachute will be a significant step toward modeling the fluid structure interaction for opening parachutes.




*Computed streamlines for a steady simulation at a Reynolds number of 1 million. Parachute surface and streamlines are colored based on the computed pressure field.*

# CFD as a Tool to Authorize Flight Test

S.B. Kern and D.B. Findlay
*Naval Air Warfare Center, Aircraft Division, Warminster, PA*

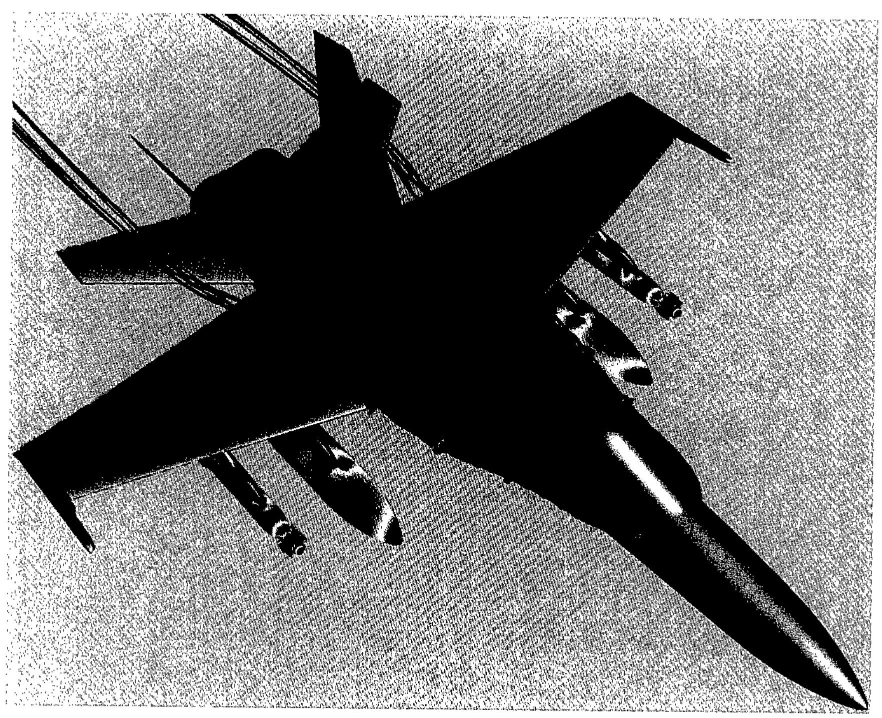
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To provide distributed aerodynamic loads on the Joint Direct Attack Munition (JDAM) at captive carriage on the F/A-18C outer-wing pylon for subsequent structural evaluation and flight test within a three-week time period.

***Methodology:*** An overset Navier-Stokes flow solver, OVERFLOW, was applied to the full-configuration F/A-18C with external fuel tanks and the JDAM weapon at captive carriage on the outer wing pylon. The computational grid of the configuration had more than 3 million computational cells. The Euler equations were solved over the aircraft, and the thin-layer Navier-Stokes equations with an algebraic turbulence model were solved over the weapon at critical flight test conditions. Integrated forces and moments were correlated to wind tunnel experiments. The entire CFD analysis was performed in three weeks, including acquisition of the JDAM geometry, grid generation, and four flow solutions at critical flight conditions.

***Results:*** Integrated forces and moments of the JDAM weapon at transonic and supersonic speeds were within 10 percent of wind-tunnel-predicted results. The distributed loads were used to conduct a structural analysis to determine root bending and torsional moments of the weapon's control surfaces. It was determined that the loads were within allowable limits.

***Significance:*** The results were used to authorize a subsequent successful flight test. CFD was the only viable way to authorize this test in the required time frame because typical wind tunnel models of captive weapons do not have instrumentation to measure distributed surface pressure. This represents a major step toward integrated modeling and test environments in DoD.



*F/A-18C with pressure on the JDAM weapon surface and vortices shedding from the strake at Mach 0.95*

# SADARM Submunition Collisions

J. Sahu, K.R. Heavey, and C.J. Nietubicz
*Army Research Laboratory, Aberdeen Proving Ground, MD*

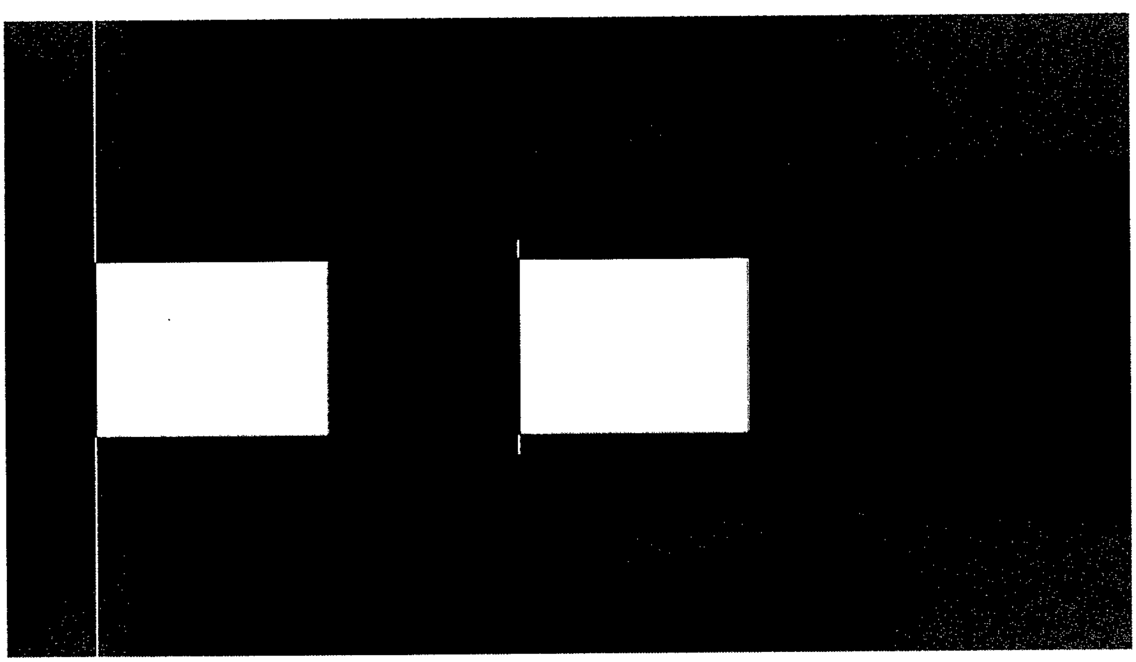
***Computer Resource:*** Cray C916 and Cray Y-MP [CEWES MSRC]

***Research Objective:*** To develop a computational capability to compute the aerodynamics of complex multibody configurations and bodies in relative motion.

***Methodology:*** This research involves application of the versatile Chimera numerical technique to time-dependent, multibody configurations. This unique multidisciplinary work couples the solution of the Navier-Stokes equations, which govern fluid motion, to the solution of the six-degrees-of-freedom equations of motion, which govern projectile flight trajectories. The Chimera technique, which is ideally suited to this problem, involves generating independent grids about each body and then oversetting them onto a base grid to form the complete model. With this composite overset grid approach, the unsteady aerodynamics associated with the bodies in relative motion can be determined without the need to re-grid. Current efforts are directed at developing a scalable, parallel version of the code on the SGI Power Challenge Array at the ARL MSRC in order to compute effectively three-dimensional configurations.

***Results:*** This advanced technology was used to provide a computational fluid analysis to a high-priority Army SADARM (Sense and Destroy Armor) program. The CFD modeling has provided physical insight into the complex unsteady flowfield associated with the SADARM submunitions during the separation/-ejection process and has helped in the evaluation of design changes.

***Significance:*** This work represents a major increase in capability for determining the aerodynamics of multiple-body configurations in a timely and cost-effective manner. The technology developed is additionally applicable to other Army problems such as time-dependent sabot separation for kinetic energy rounds, segmented rods, Multiple Launch Rocket Systems (MLRS), parachute clusters, submunition dispersal, and maneuvering projectiles.



*Mach contours showing separation of submunitions and collision avoidance, based on CFD simulation of design modifications.*

# Vortex Flow in Propeller Rotor Passage

Y.-T. Lee
*Naval Surface Warfare Center, Bethesda, MD*

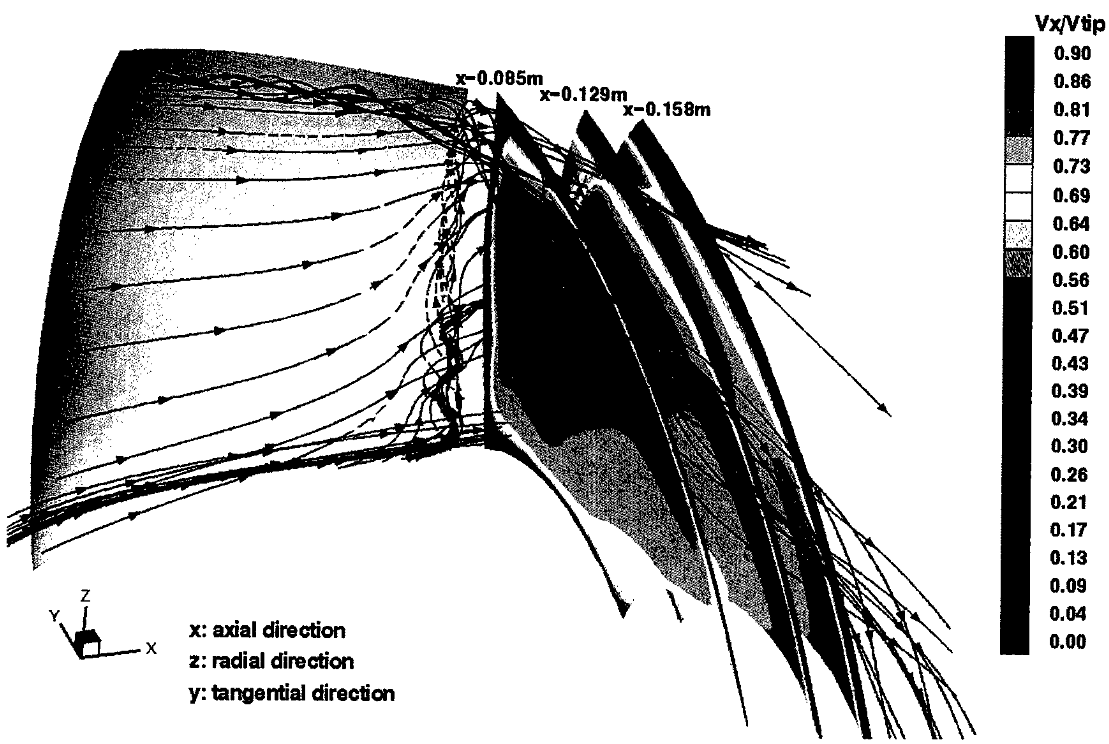
***Computer Resource:*** Cray C916 and Cray Y-MP [NAVOCEANO MSRC and CEWES MSRC]

***Research Objective:*** To simulate complex flows through marine propulsors with multiple-stage stator-rotor configurations. The detailed simulation results lead to the identification of flow-induced noise sources and predict their propagation.

***Methodology:*** The steady incompressible form of the Reynolds-averaged Navier-Stokes equations is solved with a pressure-based implicit relaxation method using a fully conservative control volume approach. A standard two-equation turbulence closure is modified to include a low-Reynolds-number model in order to integrate the governing equations up to solid walls.

***Results:*** The numerical calculation demonstrates its ability to predict the complex vortex flow pattern within the rotor passage. As shown in the figure, the fluid particle traces near a typical propeller suction surface highlight the spanwise trailing-edge separation vortex and the chordwise tip-clearance vortex from the pressure side to the suction side. The strong interaction between the trailing-edge vortex and the tip vortex is also demonstrated near the rotor tip and at the trailing-edge area.

***Significance:*** The ability to predict accurately complex propulsor flows is essential in future design processes for meeting hydrodynamic and hydroacoustic performance requirements. The validated prediction method is capable not only of providing detailed flow features inside the blade passage, but also of reducing experimental cost during design consideration.




*Flow traces on rotor blade and wake planes*

# Tiltrotor Aerodynamics Using Scalable Software

R. Strawn, R. Meakin, E. Duque, and W.J. McCroskey
*Army Aeroflightdynamics Directorate, Moffett Field, CA*

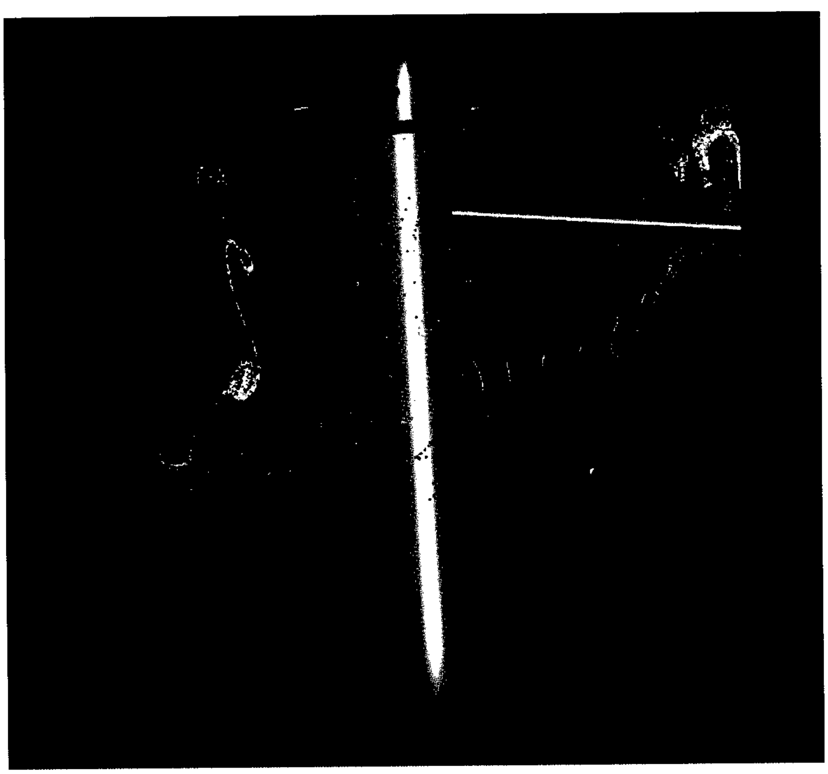
***Computer Resource:*** Cray C916 [NASA-Ames] and TMC CM-5 [AHPCRC DC]

***Research Objective:*** To increase the mission effectiveness and reduce the noise, vibrations, and design cycle costs of future advanced rotorcraft. This requires validated, faster, and more reliable design and analysis codes for the aerodynamics and acoustics of complex rotorcraft configurations.

***Methodology:*** Advanced computational fluid dynamics codes are being developed that exploit the advantages of an overset grid, or "Chimera," algorithm. This technique decomposes the aerodynamic flow field around a rotorcraft into a number of geometrically simple, overlapping grid zones associated with the various components. This is essential, for example, for treating the relative motion between the rotor blades and the airframe. The flow past each component is then computed using an efficient, implicit, three-dimensional unsteady Navier-Stokes algorithm. Preliminary calculations on Cray C916 and Connection Machine CM-5 supercomputers show that scalable parallel computing technology is essential for solving large problems such as complete rotorcraft.

***Results:*** The aerodynamic "fountain effect" of the V-22 Osprey tiltrotor aircraft in hover (see figure) has been simulated and satisfactorily compared with experiments. The results provide insight into the unsteady airloads and noise generated during landing.

***Significance:*** The ability to simulate accurately the aerodynamics and acoustics of rotorcraft allows quieter and more efficient military and civilian vehicles to be designed at lower cost and less risk. Analysis of the computed flow separation on the airframe of the V-22 aircraft has already helped the manufacturers avoid costly redesign errors as they sought to improve high-speed performance. Also, it has documented the highly three-dimensional and unsteady nature of the fountain effect in hover.



*Particle traces show the unsteady flowfield for the V-22 tiltrotor and wing*

# Store Separation Using Dynamic CFD Simulations

W.C. Riner and D.M. Cline
*Sverdrup Technology, Inc., Eglin Air Force Base, FL*
J.M. Brock
*Eglin Air Force Base, FL*
*Air Force Development Test Center, Eglin Air Force Base, FL*

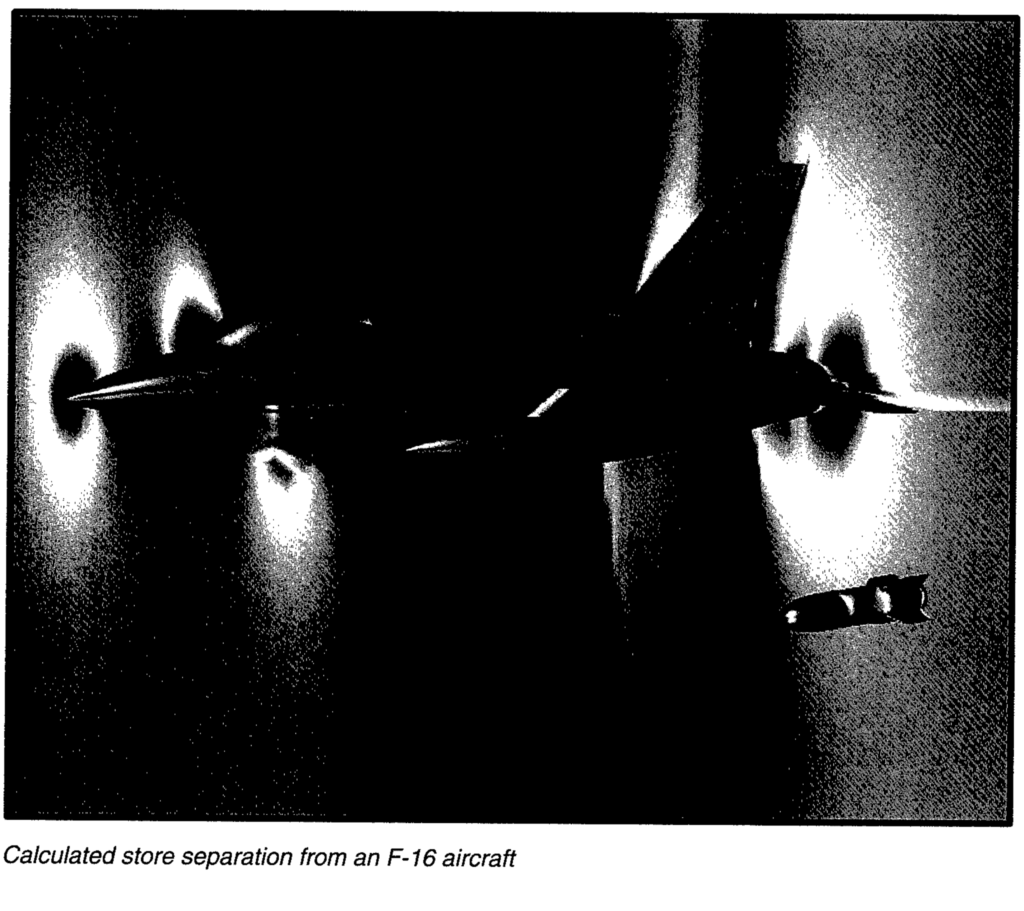
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC and CEWES MSRC] and Cray T3D [AFDTC DC]

***Research Objective:*** To predict the separation trajectories of stores from Air Force aircraft using dynamic CFD methods. Fuel tanks, bombs, and missiles attached to the undercarriage of airplanes are called stores. Accurate prediction of the motion and rotation of these stores as they separate from the aircraft is critical for flight safety.

***Methodology:*** A time-accurate CFD method combined with a dynamic simulation is used to calculate the trajectories of stores after release or jettison. The CFD method and dynamic simulation are contained in a single computer code. A preliminary multiprocessing version has been implemented on the Cray T3D.

***Results:*** Computed trajectories of these stores have been successfully verified against wind tunnel measurements.

***Significance:*** Traditional wind tunnel methods use an approximate quasi-steady method to predict store motion. The simulation method uses a time-accurate method. Simulation of store trajectories will reduce the need for expensive and time-consuming ground and flight testing.



*Calculated store separation from an F-16 aircraft*

# Missile Aerodynamics

S. Aliabadi, C. Waters, and T. Tezduyar
*ARL/Army High Performance Computing Research Center, Minneapolis, MN*
S. Ray and W. Sturek
*Army Research Laboratory, Aberdeen Proving Ground, MD*

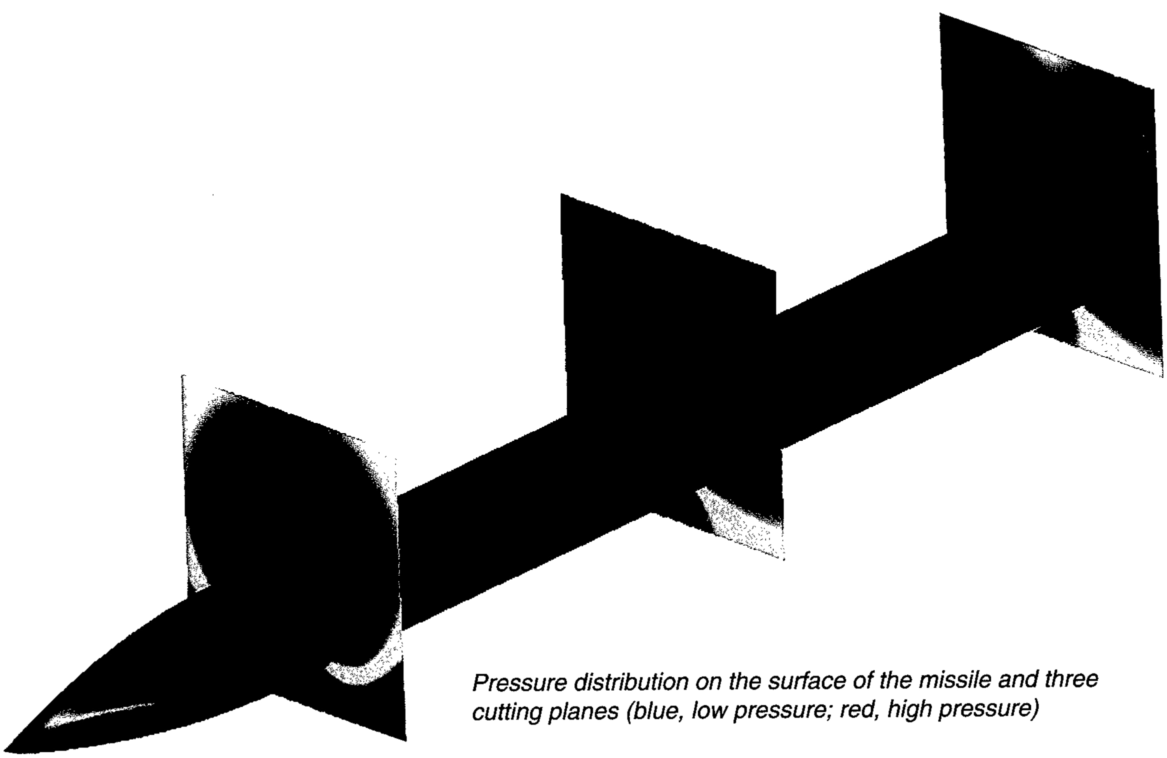
***Computer Resource:*** Cray T3D [AHPCRC DC]

***Research Objective:*** To evaluate Navier-Stokes computational techniques for the prediction of separated flow fields around high-length-to-diameter bodies at moderate angles of attack and supersonic velocities. The compressible flow solver developed by the researchers at the Army High Performance Computing Research Center is used in this research.

***Methodology:*** The compressible Navier-Stokes flow solver is based on the stabilized finite-element formulation in the context of conservation variables. This three-dimensional flow solver, which allows the use of unstructured meshes, has been implemented on the massively parallel Cray T3D supercomputer using PVM libraries. To prevent excessive memory demands, a matrix-free iterative solver is used to solve the coupled nonlinear equations resulting from the implicit formulation.

***Results:*** The turbulence effect around the missile is studied on the Cray T3D. The free-stream Mach number is 2.5, angle of attack is 14 degrees, and Reynolds number based on the diameter of the missile is 1.2 million. The finite-element mesh used in this computation consists of 918,000 hexahedral elements and 944,366 nodes, resulting in more than 4.5 million coupled nonlinear equations. Comparison between computed and experimental results is quite satisfactory.

***Significance:*** The capability of numerically simulating the aerodynamics of missiles with high accuracy on parallel architectures reduces the design cost of future generations of missiles.



*Pressure distribution on the surface of the missile and three cutting planes (blue, low pressure; red, high pressure)*

# Advanced Compact Inlet Systems

Lt. J.D. Hank, U.S. Air Force
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

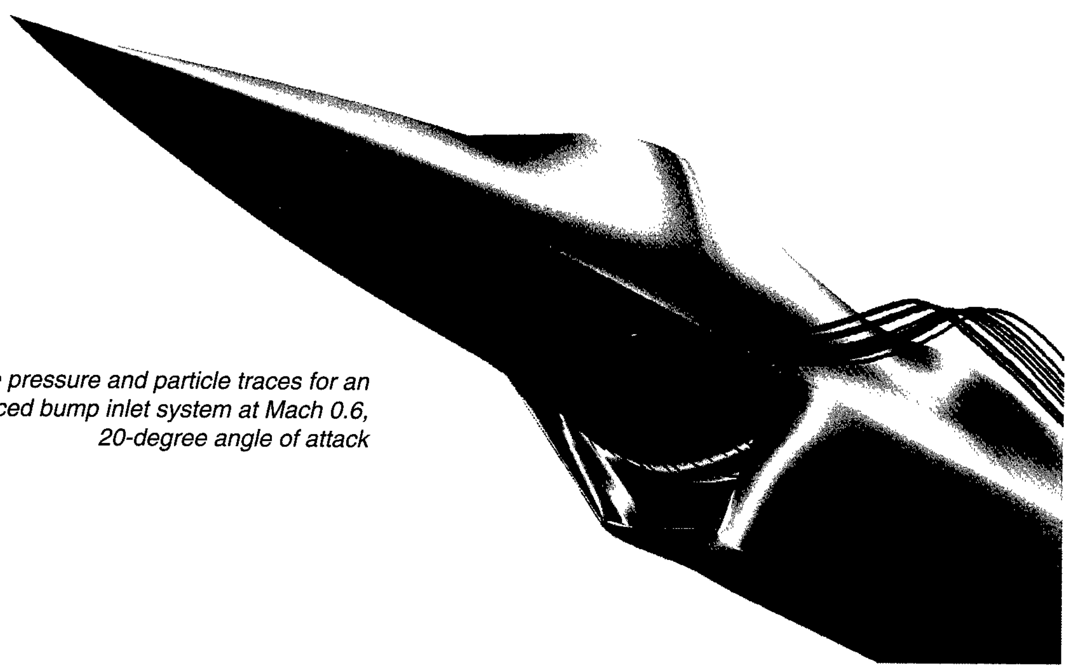
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC]

***Research Objective:*** To increase understanding of the complex flowfield characteristics of compact inlet systems. Potential problem areas investigated include forebody-chine vortex ingestion, compression surface boundary-layer removal efficiency, and flow separation in highly offset serpentine diffusers.

***Methodology:*** Viscous flow is simulated around a forebody-inlet configuration at a variety of flow conditions to evaluate inlet system performance. Solutions were generated using Cobalt, an unstructured finite-volume code developed at Wright Laboratory. Cobalt is based on Godunov's Riemann method and uses the Spalart-Allmaras turbulence model to simulate the fine-scale effects of turbulence. The Cobalt results will be compared with a state-of-the-art structured, finite-difference solver to compare accuracies and resource savings.

***Results:*** Flow separation and poor corner-flow regions have been identified in the serpentine diffuser. Inlet system performance data have been obtained at various flight conditions. These will be compared and verified against future experimental data.

***Significance:*** Traditional inlet design tools are not applicable to current advanced inlet concepts. CFD has been shown to be a useful tool in advanced inlet design by allowing propulsion engineers to visualize the complex, three-dimensional nature of advanced inlet flowfields. The computational results will supplement experimental data and greatly enhance the design database for compact inlet systems. Additionally, numerical screening of inlet concepts allows inlet designers to better utilize limited testing resources by testing only the most promising designs.



*Surface pressure and particle traces for an advanced bump inlet system at Mach 0.6, 20-degree angle of attack*

# Supersonic Flow over a Missile Body at High Angle of Attack

D. Kinsey and E. Josyula
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

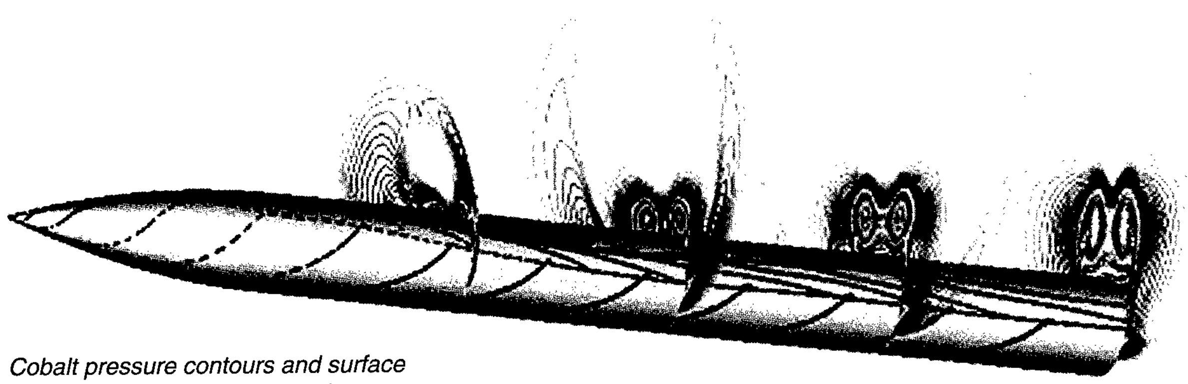
***Computer Resource:*** Cray C916 [CEWES MSRC and NAVOCEANO MSRC]

***Research Objective:*** To determine the predictive capability of Navier-Stokes solvers on the complex vortical flow around a missile body in supersonic flow at high angles of attack. This rather-simple shape produces complex flow physics that challenge the capability of current flow solvers and turbulence models.

***Methodology:*** Each author used a separate flow solver and turbulence model. The first flow solver, Cobalt, is an unstructured, finite-volume, cell-centered, Riemann solver based on Godunov, but with the approximate method of Collela, in combination with the iterative method of Gottlieb and Groth. Second-order accuracy in space for the inviscid terms is patterned after van Leer's MUSCL scheme, while the viscous terms follow the work of MacCormack. Up to fourth-order accuracy in time is achieved via the low-storage Runge-Kutta method of Williamson. The Spalart-Allmaras turbulence model was used. The second flow solver, FDL3DI, is a structured, implicit, approximate-factorization Beam-Warming algorithm. The spatial terms are central differenced, second-order accurate. Turbulent effects are included using a $k$-$\varepsilon$ turbulence model.

***Results:*** The CFD results were compared with experimental data from a wind tunnel test of a sting-mounted model approximately 4 feet long and 3.7 inches in diameter. The test conditions were Mach 2.5, 14 degrees angle of attack, and a Reynolds number of 4 million per foot. Surface static pressure and pitot pressure contour data were obtained at several stations along the missile. All of the important flow structures were correctly captured with both flow solvers and their respective turbulence models. The surface static pressures correlated quite well, with only a small error in the region after initial separation. The pitot pressure contours compared well with experiment in shape and location; however, the predicted pressures in the vortex core were not as low as in the experiment.

***Significance:*** This work was part of a collaborative study between Canada, the United Kingdom, and the United States, with Army, Navy, and Air Force organizations participating for the U.S. Eight separate Navier-Stokes codes, representing a wide variety of methods and turbulence models, provided tremendous insight into the current state of the art in CFD.



*Cobalt pressure contours and surface streamlines for Mach 2.5, 14-degree angle of attack*

# V-22 Aircraft Tail Buffet Aerodynamics

T.C. Tai
*Naval Surface Warfare Center, Bethesda, MD*

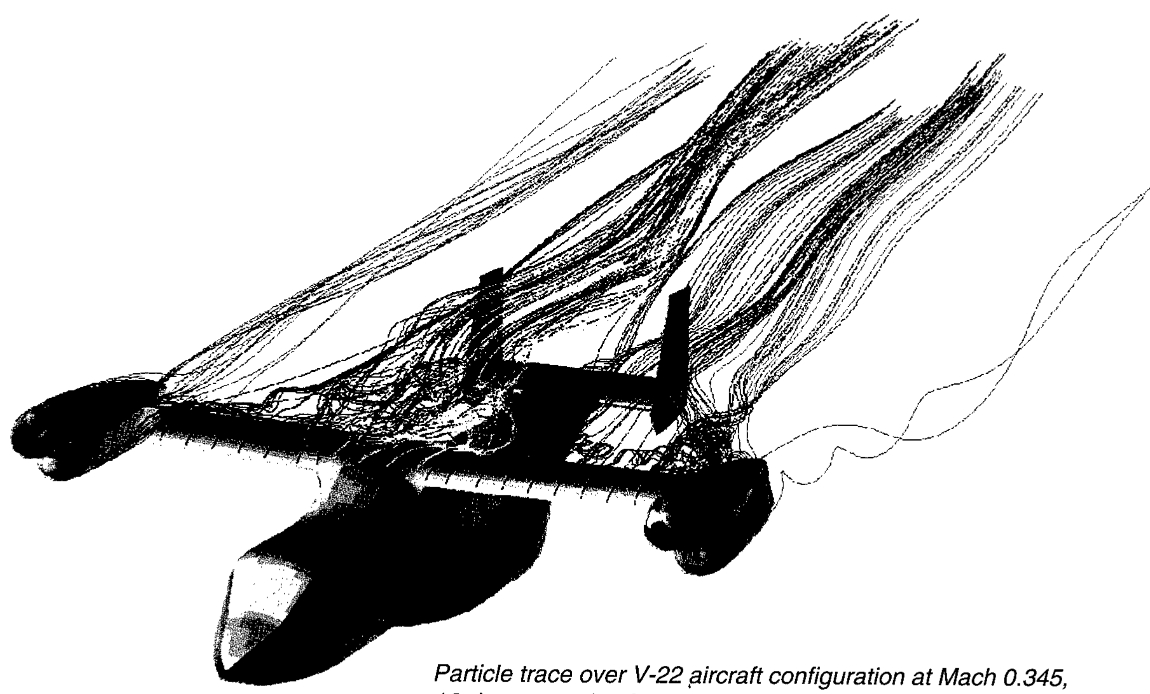
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC and CEWES MSRC]

***Research Objective:*** To investigate the V-22 aircraft tail buffet aerodynamics in support of the Navy's V-22 Tiltrotor Aircraft Development program.

***Methodology:*** A multizone, thin-layer Navier-Stokes method is used to simulate the flow field about the V-22 aircraft configuration in forward-flight mode at high angles of attack. The steady-state flowfield is analyzed for possible onset of a vortex breakdown somewhere before the tail section. The NASA CFL3D code is used as the flow solver. This code solves the three-dimensional (3-D) Reynolds-averaged Navier-Stokes equations through a finite-volume scheme.

***Results:*** Computations were performed for flow over a V-22 aircraft configuration at several high angles of attack at a freestream Mach number ranging from 0.345 to 0.45. A new successive multiblock grid-generation scheme is developed in generating the desired grid for this complex geometry. Analysis of the simulated flowfield is focused on one of the two primary factors that affect the onset of vortex breakdown: the swirling of the flow attributed by the 3-D flow separation on the upper wing surface. The figure shows the particle trace from the simulated flowfield. Flow separation over the upper wing surface is massive, and large crossflows flowing in-board toward the fuselage are apparent. The crossflow mixes with the main stream over the fuselage, contributing to the swirling of the flow as it proceeds downstream. Because of the intensity of flow swirling and the large adverse pressure gradient, the vortex bursts between the midwing fairing and the horizontal tail. This onset angle of attack agrees with flight-test data.

***Significance:*** The ability to detect the onset of vortex breakdown allows the aerodynamics design engineer to apply advanced control techniques to defer or relocate the vortex bursts. This ability to modify the tail buffeting translates into an increased range of flight conditions in which the aircraft can be operated effectively.



*Particle trace over V-22 aircraft configuration at Mach 0.345, 16-degree angle of attack, and 10-degree sideslip angle*

# Compressor Stall Simulation

R.A. Adomaitis
*University of Maryland, College Park, MD*
*Air Force Office of Scientific Research, Washington, DC*

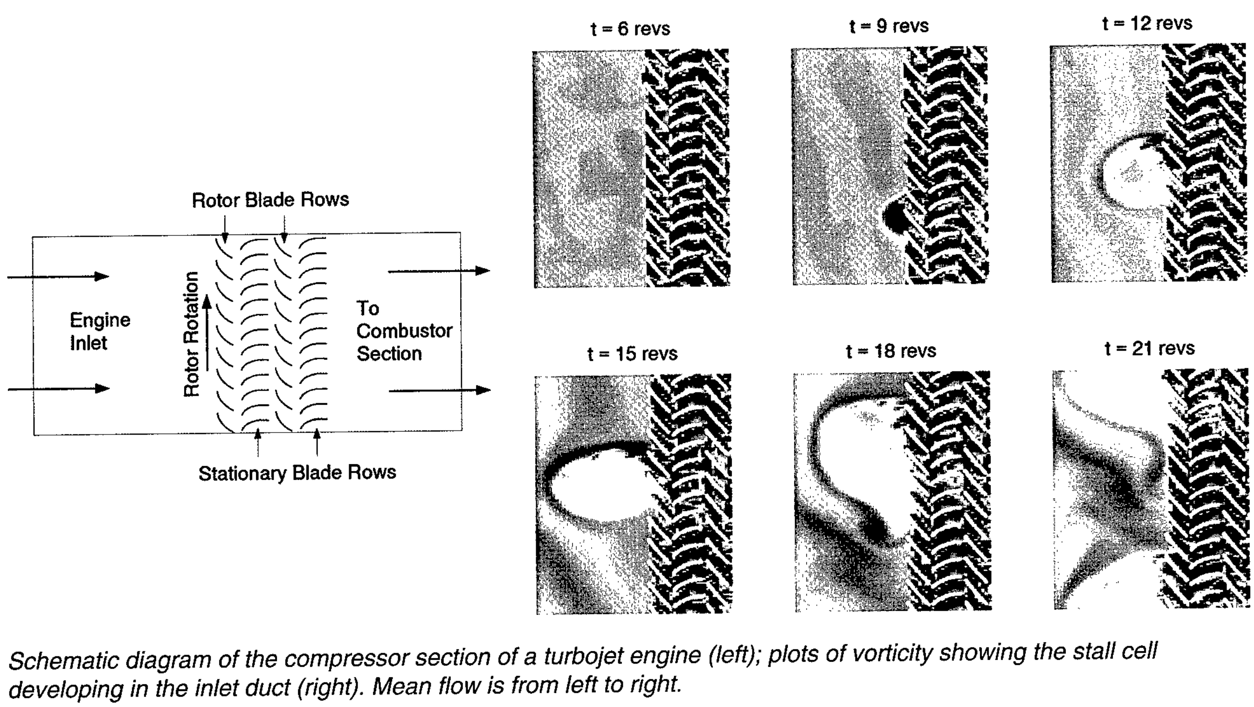
***Computer Resource:*** TMC CM-5 [AHPCRC DC]

***Research Objective:*** To develop a dynamic simulator capable of predicting compressor stall in gas turbine aero-engines as part of a research program focusing on nonlinear analysis and control of compression system flow instabilities.

***Methodology:*** Computations consist of direct, two-dimensional numerical simulation of the air flow through the compressor, inlet/exit ducting, and the throttle valve. Forcing functions to the Navier-Stokes equations replace rotor and stator blade boundary conditions, so computations are performed over a simplified domain. This approach was chosen specifically for the TMC CM-5 to maximize the ratio of nearest-neighbor to routed communications and to allow the use of fast and memory-efficient Poisson-type equation solvers.

***Results:*** Stall inception predictions corroborate with experimental observations of flow instabilities in multistage compression systems. Simulation methods developed are well-suited to model reduction for bifurcation analysis.

***Significance:*** Compressor stall is an inherent performance limit and safety issue in all gas turbine engines. The simulator developed predicts these events with fidelity sufficient to study instability inception, compare control techniques, and evaluate sensor placement and signal processing methods for stall precursor detection.




*Schematic diagram of the compressor section of a turbojet engine (left); plots of vorticity showing the stall cell developing in the inlet duct (right). Mean flow is from left to right.*

# Simulation of Flow Past a Swimming Tuna

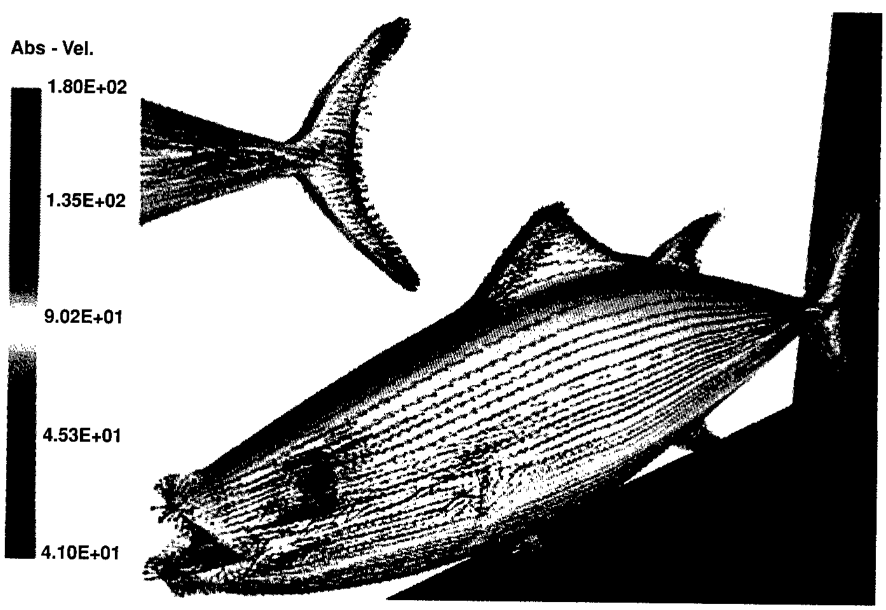
R. Ramamurti and W.C. Sandberg
*Naval Research Laboratory, Washington, DC*
R. Löhner
*George Mason University, Fairfax, VA*

***Computer Resource:*** Cray C916 [CEWES MSRC and NAVOCEANO MSRC]

***Research Objective:*** To perform three-dimensional (3-D) numerical simulations of incompressible flows based on unstructured grids. This model is one of the DoD HPC benchmark codes. The flow solver is combined with adaptive remeshing techniques for transient problems with moving grids and is also integrated with the rigid body motion in a self-consistent manner. This allows the simulation of fully coupled fluid-rigid body interaction problems of arbitrary geometric complexity in three dimensions. This flow solver has been successfully used in the past for simulating torpedo launch from a submarine.

***Results:*** Three-dimensional flow past a tuna with an oscillating caudal fin was simulated. The motion of the caudal fin was prescribed. Several steady-state solutions were obtained at various caudal positions during one quarter of a cycle. The capability of the flow solver to compute flow past deformable bodies was demonstrated via an unsteady flow simulation for three cycles. The force generated by the caudal fin and the body were computed and compared to the steady-state simulations. It was clear that the steady-state simulations could capture neither the magnitude nor the trend of the variation of forces observed in the unsteady simulations.

***Significance:*** This represents a new capability for computing flow past deformable and moving surfaces. Significant potential exists for the design of novel and efficient control surfaces for maneuvering underwater vehicles of interest to the Navy. Autonomous "swimming" vehicles being considered for coastal defense and similar propulsion concepts show great promise for ultrasmall aircraft.




*Flow past a swimming tuna with caudal fin oscillation. The velocity vectors on the surface show a low velocity region extending from the mouth along the centerline and a small recirculating region (shown in the inset) near the peduncle region.*

# Tip Vortex Generated by a Propeller

L.L. Pauley, C.T. Hsiao, and P.G. Wilson
*The Pennsylvania State University, University Park, PA*
*Office of Naval Research, Arlington, VA*

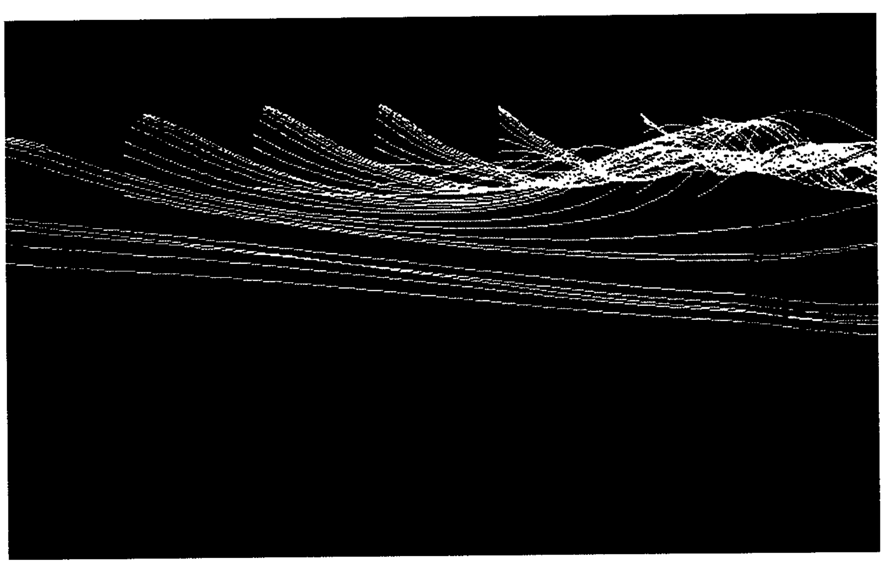
***Computer Resource:*** Cray C916 and Cray YMP [CEWES MSRC and NAVOCEANO MSRC]

***Research Objective:*** When a flow passes over a finite-span lifting wing, a tip vortex will form as a result of the pressure difference between the pressure and suction side. The tip vortex flow field is complex, three-dimensional (3-D), and viscous, with large secondary velocities. The present study computationally investigates the tip vortex flow and 3-D separation near the tip of a hydrofoil.

***Methodology:*** Incompressible Navier-Stokes computations are used to describe accurately all phenomena present in the tip vortex flow. Both one-equation turbulence models and large-eddy simulations (LES) have been tested. Before executing the full Navier-Stokes computation, an appropriate 3-D grid generation was developed to consider the complex flow field and tip geometry. Because of the complexity of LES, this method was tested for 2-D and 3-D computations in the simplified geometry of a flat surface with imposed 2-D external pressure gradient. Two different subgrid scale models, the constant Smagorinsky model and the dynamic subgrid scale model, were investigated.

***Results:*** The 3-D incompressible Navier-Stokes solver (INS3D) is used to numerically simulate the flow around the finite-span wing. Steady state computations have been completed at several Reynolds numbers and angles of attack. A swept hydrofoil geometry was also tested. Present efforts include unsteady computations. The current research applies LES to transitional separation bubbles produced by an adverse pressure gradient, which was uniform across the span. Two-dimensional and three-dimensional LES were conducted and the results compared with experimental measurements. Both 2-D and 3-D computations captured the time-averaged structure and pressure coefficient distribution measured in experiments. The 3-D computations demonstrated the strongly 2-D separation structure that was observed experimentally.

***Significance:*** This study investigates the 3-D separation and tip vortex generated in a propeller geometry. By understanding the structure of this flow, conditions that produce cavitation inception can be better predicted and prevented. Cavitation should be minimized in propeller design because it causes noise and blade erosion.



*Particle trace of a tip vortex generated by a rectangular planform NACA 0015 hydrofoil at 12 degrees angle of attack and Reynolds number of 1,500,000.*

# Elimination of Explosions and Propellants Through Safe Open-Air Detonations

C.A. Lind, T.R. Young, Jr., A.M. Landsberg,
E.S. Oran, and J.P. Boris
*Naval Research Laboratory, Washington, DC*
W. Mitchell
*Environmental Protection Agency, RTP, NC*
C. Biltoft
*Army Dugway Proving Ground, UT*

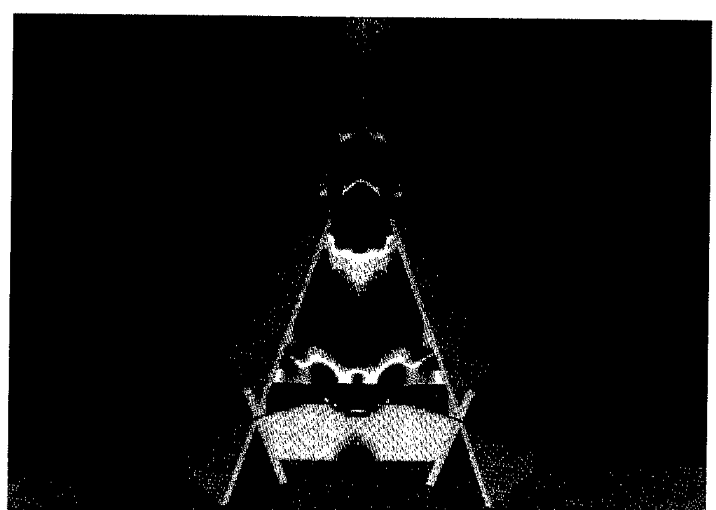
***Computer Resource:*** Intel Paragon XP/S-15 [ASC MSRC] and Intel iPSC/860 [NRL DC]

***Research Objective:*** To develop a methodology for permitting the in-place detonation of expired and obsolete munitions in the safest and most environmentally sound and cost-efficient manner to remove these hazards.

***Methodology:*** The CFD simulation code FAST3D is being used to characterize the explosion sources in containment facilities with terrain as input to a NOAA atmospheric dispersion model. The source characterization model requires describing the relevant parameters of the detonation processes (such as the propagation and intensity of the blast wave and acoustic overpressures), the type and amount of the solids and other pollutants released, afterburn in and water quenching of the fireball, and the resulting plume buoyancy and dimensions as a function of time.

***Results:*** Simulations have been performed of several proposed design options. These have highlighted problems including shock focusing and noise. Considerations in the design loop include the position, size, and shape of the explosion as well as the shape of the containment facility. The design of the containment facility can be analyzed through these simulations to minimize the shock focusing, thus reducing the loads on the structure. The design considerations also include minimizing the far-field noise and maximizing the afterburn of explosion byproducts.

***Significance:*** Safe elimination of obsolete explosives with minimal environmental impact and maximal savings is a major DoD objective, being a necessary prerequisite for base reductions and re-use of land resources. Computer simulation is being used to design the complex open-air detonation structures constructed of steel-clad flat and curved prestressed concrete. Savings of more than $1 billion are projected for removing obsolete explosives alone, more than $2000 per ton for the half million tons of obsolete explosives now in the U.S. inventory. The flash incineration approach is equally promising for destruction of biological and chemical weapon materials, currently a $12 billion program.



*Potential octagon design of a containment facility for open-air detonation of expired and obsolete munitions*

# Development of a Coupled CFD/CSD Methodology

J.D. Baum and H. Luo
*SAIC, McLean, VA*
R. Löhner
*George Mason University, Fairfax, VA*
*Defense Nuclear Agency, Alexandria, VA*

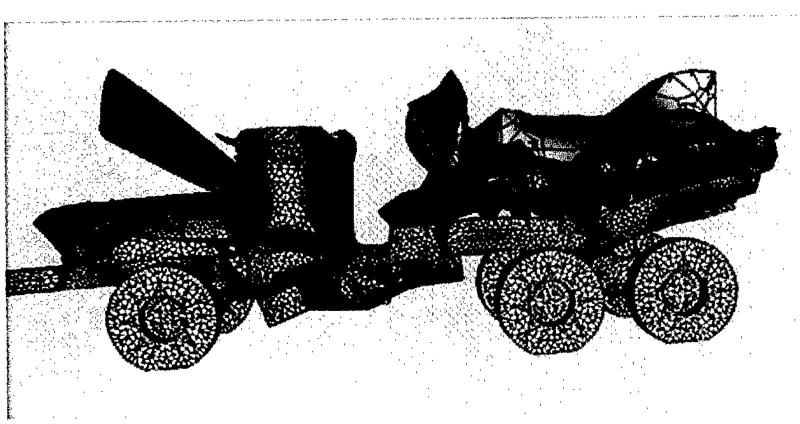
***Computer Resource:*** Cray C-90 [CEWES MSRC] and Cray YMP-8/2048 [Los Alamos National Laboratory, NM]

***Research Objective:*** To develop a novel, fully integrated, computational fluid dynamics (CFD) and computational structural dynamics (CSD) methodology for transient simulations. This methodology provides the simultaneous determination of the free-field propagation of blast waves initiated by either conventional or nuclear weapons, the loads exerted on the structures by the impinging shocks, the structural deformation and kinematic motion, and the resulting modifications to the flowfield. Past methodologies applied either an iterative approach or a completely decoupled approach, leading to time-delays, loss of information, and most importantly, loss of insight. The new methodology significantly reduces turnaround time and the probability of analysis error, increasing our understanding of the problem and enabling the simulation of new classes of problems.

***Methodology:*** Fully integrated state-of-the-art CFD and CSD algorithms are combined. The CFD methodology, FEFLO97, is a recently developed three-dimensional, adaptive, finite-element, edge-based, arbitrary Lagrangian/Eulerian shock-capturing methodology based on unstructured tetrahedral grids. It is used for solving the Euler and Reynolds-averaged turbulent Navier-Stokes equations. FEM-FCT is a high-resolution monotonicity-preserving algorithm. The CSD methodology, DYNA3D, uses unstructured grids and a spatial discretization that involves finite-element techniques, large deformation formulation for the solids, explicit time integration, and several material models, kinematic options, and equations of state.

***Results:*** The developed methodology has been successfully applied to both military and civilian applications. Military applications include blasts in underground shelters, where pretest predictions were in very good agreement with available experimental data, and blast interaction with military equipment (trucks and tanks). Civilian applications include the study of the blast in the World Trade Center. The coupled methodology has provided understanding and improved prediction of both shock wave diffraction phenomena and structural response to blast loading.

***Significance:*** The coupled methodology significantly enhances the survivability and hardness evaluation of military equipment and blast damage to underground command and control centers and other targets of military significance. Simultaneously, the methodology provides cost-effective evaluation of civilian structures hardening against terrorist attacks.



*Computational structural dynamics mesh on the deformed surface of a standard 5-ton Army truck carrying a command and control center*

# Coupled Explosion-Structure Interactions

P.A. Hookham and V.E. Koik
*Titan Research and Technology, Chatsworth, CA*
*Defense Nuclear Agency*

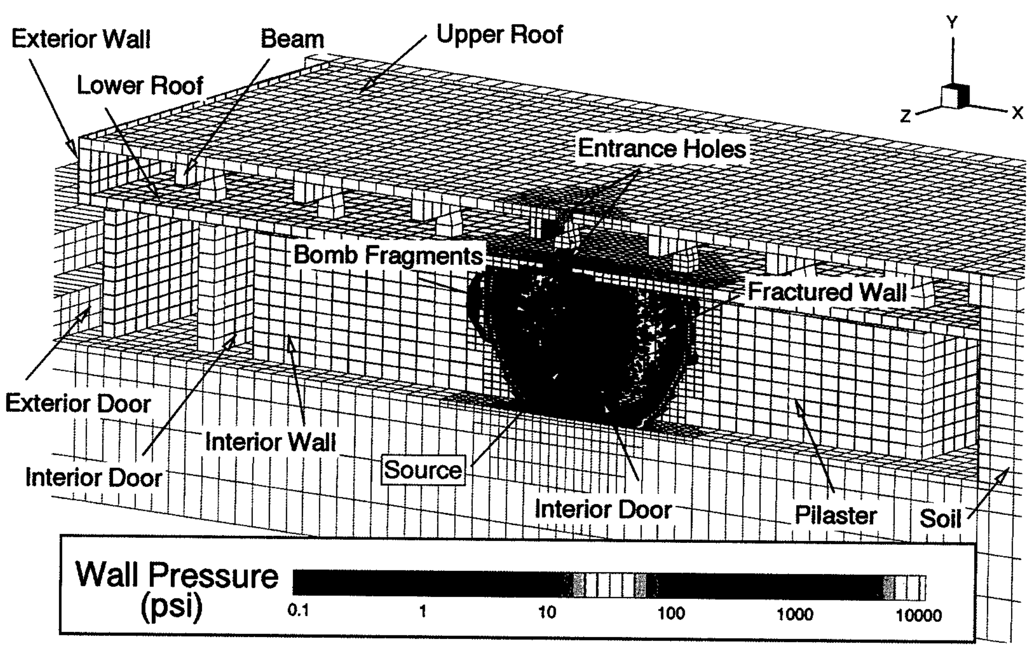
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC]

***Research Objective:*** To develop and validate a computational fluid and solid dynamics (CFSD) methodology capable of simulating highly transient fluid-structure interactions involving large deformations and structural failure.

***Methodology:*** The TRT MAZe (multiphase, adaptive zoning) CFSD code solves the continuum equations of motion for multiple material regions or multiple phases in a single computational cell. For fluid regions, the Reynolds-averaged Navier-Stokes equations are solved using a high-order finite-volume, total variation-diminishing, monotonicity-preserving numerical scheme. For solid material regions, elastic-plastic equations of state are solved using a similar numerical approach. Solid material cells may fail when reaching a predefined failure criterion, such as a strain limit, and the cell is then converted into a multiphase cell (with rubble and air, e.g.). The code also contains subroutines for modeling solid materials using finite-element structural approaches (beam or plate elements, e.g.). Automatic adaptive zoning optimizes the resolution of user-specified gradients in the solution.

***Results:*** The methodology was used to perform a pretest prediction of a field test in which a high-explosive bomb was detonated within a relatively weak multiroom structure with concrete block walls. The simulation accurately reproduced the massive structural deformation and failure that occurred in the test. The code also predicted overpressure time-histories that were in good agreement with measured values, even in gauge locations that required accurate modeling of the failure of walls between the bomb and the pressure gauge.

***Significance:*** This methodology substantially improves conventional decoupled fluid-structure calculations for predicting explosion-structure interactions where substantial structural deformation and failure occur.




*Three-dimensional MAZe CFSD simulation of a bomb detonation in a structure (air pressure contours on wall surface at 1.0 ms)*

# Inertia-Gravity Wave Breaking Simulations

J.R. Isler, D.C. Fritts, and O. Andreassen
*University of Colorado, Boulder, CO*
*Air Force Office of Scientific Research, Washington, DC*

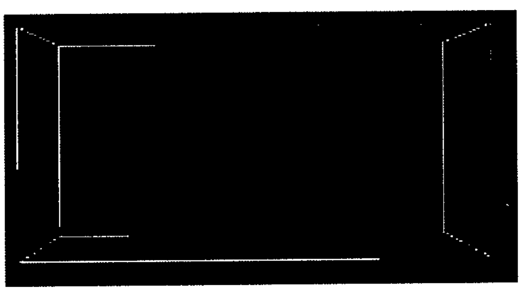
***Computer Resource:*** Cray Y-MP [NAVOCEANO MSRC] and Cray C916 [CEWES MSRC]

***Research Objective:*** To investigate the nature of internal wave breaking in the atmosphere at lower frequencies and larger spatial scales than had been simulated previously; and to investigate a range of causes for orthogonal structures in airglow, including wave superposition and inertial effects, that had not been previously included.

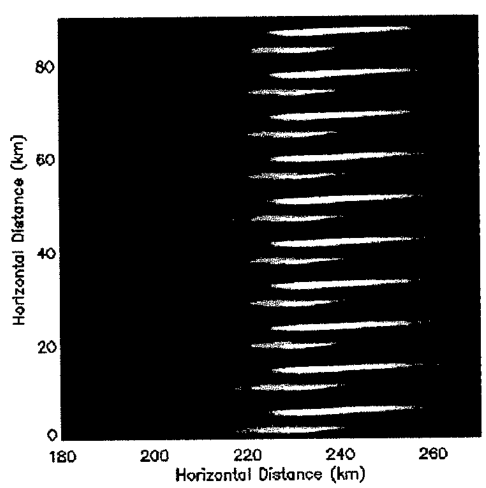
***Methodology:*** The numerical model is a two-domain three-dimensional Fourier/Chebyshev spectral model solving the Euler equations in a compressible, stratified, rotating atmosphere.

***Results:*** Recent observations of airglow emissions in the mesopause region (80-100 km) using charge-coupled device (CCD) cameras have revealed the ubiquitous nature of gravity wave activity at these heights. These cameras sometimes show small-scale bands aligned approximately orthogonal to the phase fronts of the wave. On the basis of previous nonlinear gravity wave simulations, which followed the evolution of a high-frequency gravity wave from laminar two-dimensional flow through the onset of instability to eventual isotropic turbulence, these orthogonal structures were shown to be associated with streamwise vorticity that develops as the result of the onset of convective overturning in the wavefield. The simulations presented here demonstrate that larger scale, lower frequency, breaking gravity waves also give rise to orthogonal structures in airglow images. They also demonstrate that the generation of streamwise vorticity is a characteristic signature of convective instability in wave breaking over a wide range of spatial and temporal scales.

***Significance:*** This research has led to increased understanding of airglow modulation in a breaking wave environment. This understanding is important because infrared airglow emissions are a natural background through which any space-based missile launch detection system must see.



*Eddy vorticity field after the occurrence of convective instability for a superposition of low-frequency inertia-gravity waves. Red (blue) represents positive (negative) streamwise vorticity.*




*Simulated airglow image for zenith viewing using the results of the simulation above*

# Cavity Acoustics

Capt. M.J. Lutton, U.S. Air Force
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

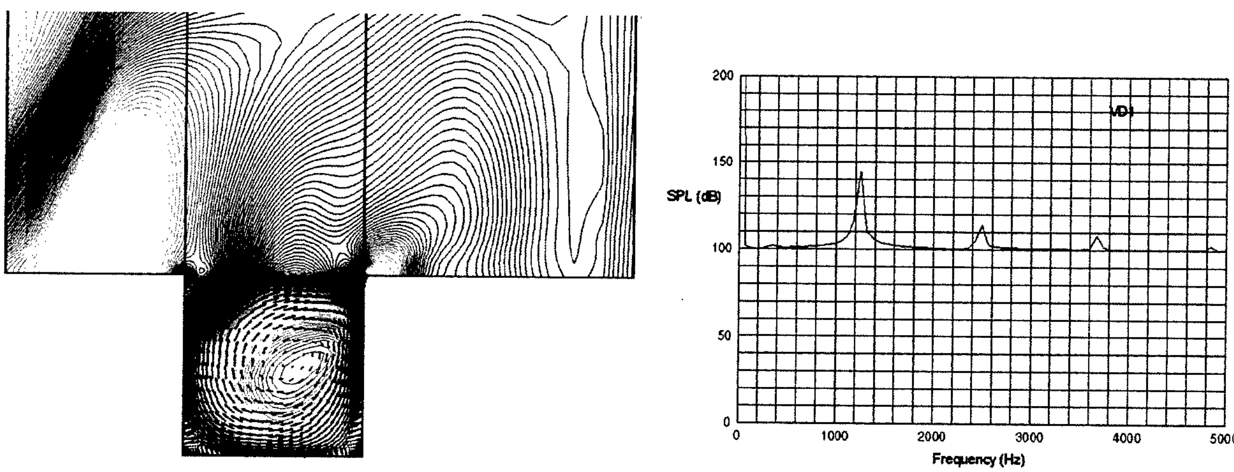
***Computer Resources:*** Cray Y-MP [CEWES MSRC]

***Research Objective:*** To examine the flow in a cavity and the attendant pressure distribution and acoustic levels. The cavity represents a hole created in the side of large civilian airliner, and is studied to quantify sound pressure levels to assess the potential for progressive structural damage.

***Methodology:*** The flows are simulated by solving the full unsteady Navier-Stokes equations using the implicit Beam-Warming algorithm and a $k$-$\varepsilon$ turbulence model. The Chimera grid overset method is used to allow optimal use of computational resources. Fourier transforms are performed on the unsteady pressures to quantify relevant frequency and amplitude information.

***Results:*** Two configurations were used: a cavity with an aspect ratio of one, and a more realistic configuration simulating the cargo hold of a typical civilian airliner. The frequency response of the sound pressure levels showed very good agreement with experiment. Some attenuation of amplitude is noted in the simulation, which is attributed to the dissipative characteristics of the turbulence model.

***Significance:*** The research was performed to assess the survivability of a large civilian airliner suffering an explosion in a cargo hold with a resultant hole in the side of the aircraft. Sound pressure levels were obtained to determine the potential impact on the structure in the immediate vicinity of the hole.




*Cavity pressure contours and velocity vectors with associated Fourier response*

# Fluid-Structure and Liquid-Gas Interactions in Liquid Propellant Guns

G. Wren and S. Ray
*Army Research Laboratory, Aberdeen Proving Ground, MD*
S. Aliabadi and T. Tezduyar
*ARL/Army High Performance Computing Research Center, Minneapolis, MN*

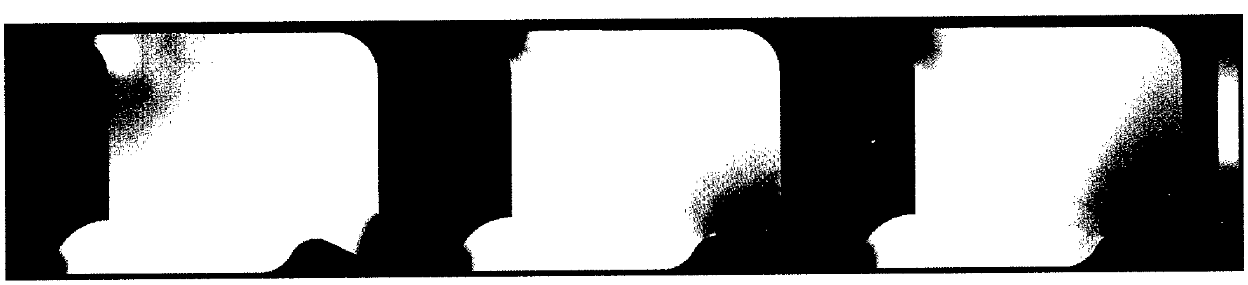
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To develop numerical tools for studying phenomena that occur in regenerative liquid propellant guns (RLPG). One area of research within the RLPG is the injection of the liquid propellant (LP) from the reservoir into the combustion chamber, and the effect of vibration of a piston within the RLPG upon the injection. The second area studied is the breakup of the LP into droplets resulting from the interaction of the LP with hot gas.

***Methodology:*** The Navier-Stokes equations for compressible flow are discretized using a stabilized space-time finite-element formulation that is capable of handling the large change in the shape of the RLPG interior as the firing cycle proceeds. It is also capable of accurately capturing the shape of the interface between the LP and the gas. To study the fluid-structure interaction problem, the fluid model is coupled to a numerical model of a deformable solid. Unstructured meshes are used and are updated within each time step using advanced mesh update strategies developed at the AHPCRC. Large linear equation systems are solved using iterative and direct solution methods.

***Results:*** The firing cycle of the RLPG is being studied to determine the effect of piston deformation on the injection of LP. Results compare favorably with experimental data obtained from test firings of the RLPG. The study of the interaction of LP and hot gas has generated interesting results that are helping to develop a more accurate model of droplet formation.

***Significance:*** These results are providing important new insights into the interaction of the injected LP and the vibrating piston during the interior ballistic process, and its impact on the fluid flow from the reservoir into the combustion chamber. Also, an understanding of the physics of droplet formation is important for studying the beginning of the firing cycle.



*Pressure distribution in the liquid propellant reservoir of the RLPG at three times during the firing cycle. The flexure of the injection piston causes a pressure fluctuation in the liquid reservoir that is moving from right to left.*

# Resonance-Generated Distribution Structures in Magnetotail X-line Configurations

J.B. Harold, G. Joyce, and J. Chen
*Naval Research Laboratory, Washington, DC*

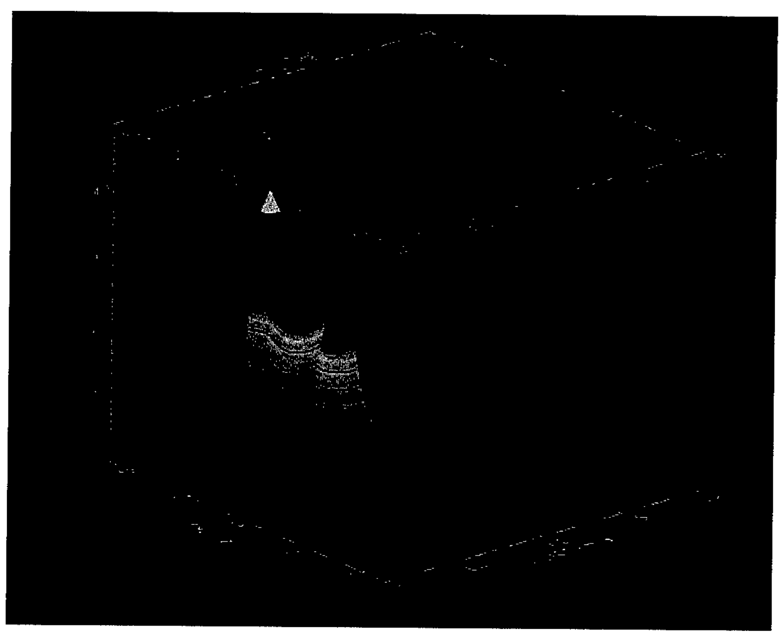
***Computer Resource:*** TMC CM-5 [NRL DC]

***Research Objective:*** To study charged particle energization in the Earth's magnetotail during disturbed times caused by solar eruptions. The results of these studies will be incorporated into general magnetospheric models.

***Methodology:*** This is one of a series of studies of plasma kinetic phenomena using a combination of modeling results from the NRL three-dimensional MHD global magnetospheric code and a kinetic particle tracking simulation code written for the NRL CM-5. The MHD code is used to generate electric and magnetic fields in the vicinity of x-lines in the Earth's magnetotail. An x-line is a region of zero magnetic field in the noon-midnight plane. Generally, these are thought to occur in response to disturbances in the solar wind.

***Results:*** We have investigated the formation of beam-like structures in the energized particle distributions, which have been reported previously. We find that in our simulations these are an x-line phenomena that can be readily explained using a simple analysis based on the phase space partitioning of one-dimensional current sheets. We confirm the expected scaling using both two- and one-dimensional models of the x-line. However, we find that the formation of these structures is critically dependent on both the field geometry and the electric field imposed at the x-line. In particular, use of an MHD-generated electric field model eliminates the energized particle population, while use of current sheets with a self-consistent width blurs the structures until they are no longer easily discernible. This calls into question the degree to which such structures obtained in previous calculations using a uniform electric field may be physical.

***Significance:*** The energization of charged particles in the vicinity of x-line formation in the disturbed magnetosphere may play a crucial role in properties and structure of the auroral zones that are important for near-Earth space phenomena, including tracking of and communication with Earth-orbiting satellites. The relationships between physically observable particle signatures and the global configuration of the magnetospheric fields are important, leading to the possibility of predicting local communications interference from global configurations.



*Particle distributions plotted as position (Z) versus velocity (V) using the full (electric and magnetic) MHD fields. The distribution was collected by a detector at 60 earth radii downstream from the Earth. The peaks near 0.2 (200 km/s) correspond to the incoming population.*

# Turbulence/Premixed Flame Interactions

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*Georgia Institute of Technology, Atlanta, GA*
*Office of Naval Research, Arlington, VA*

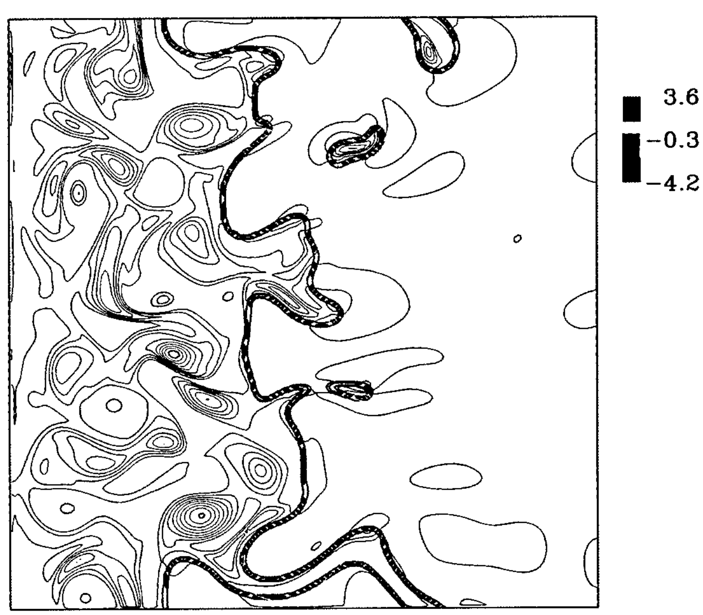
***Computer Resource:*** Intel Paragon [ASC MSRC]

***Research Objective:*** To study the propagation characteristics and structure of thin premixed flames in turbulent flows and to develop scaling rules for use in high-Reynolds-number model (large-eddy) simulation.

***Methodology:*** Direct simulations of freely propagating flames in premixed isotropic turbulence have been carried out using a FORTRAN code that solves the two-dimensional compressible Navier-Stokes equations by an explicit fourth-order accurate finite-volume algorithm. The code has been implemented using both the Intel NX and MPI message-passing libraries. The algorithm uses a domain decomposition strategy to distribute the work load to the different computational nodes. Therefore, the amount of CPU time required for a simulation is approximately inversely proportional to the number of nodes used. The size of the domain that can be simulated scales directly with the number of nodes available.

***Results:*** A snapshot of the vorticity and reaction rate contours is shown after the flame has evolved from a planar state for 2.8 large-eddy turnover times. The initial Reynolds number was 80, the ratio of the smallest turbulent scale to the flame thickness was 0.364, the ratio of the turbulent intensity to the laminar flame speed was 3.2, and the ratio of product to fuel temperature was 4. A computational grid of $800 \times 800$ on a $2\pi \times 2\pi$ domain was used for a typical simulation. Using 128 nodes on the Intel Paragon, the simulation required 25 hours, and each step required 1.54 seconds of CPU time. As the flame propagates from right to left, it is wrinkled and stretched by the turbulent field. Parcels of unburnt reactants break away from the flame and continue burning as they move downstream. Noncontinuous reaction rate contours are due to stretch effects by the turbulence. The hydrodynamic field is also altered by the presence of the flame. Heat released by chemical reaction damps the turbulent intensity and vorticity by volumetric expansion and by increasing the kinematic viscosity.

***Significance:*** Premixed flames occur in nearly all gas-turbine combustors used on Navy aircraft. The design of next-generation high-performance engines requires detailed understanding of the behavior of these flames under varying flow conditions. This will help in the development of systems to achieve robust control of the combustion processes that will enable significant reduction in infrared signature and increase reliability. For example, the recent Fixed Wing Vehicle Technology Development Approach DoD Study has mandated that infrared signature be reduced by 45 percent and reliability be increased by 50 percent for military aircraft by the year 2005.




*Premixed flame propagating into a turbulent field, showing vorticity and reaction rate (black) contours. Color map has been weighted for illustration.*

# Stability of Ram Accelerator Projectiles

C. Li, K. Kailasanath, and E.S. Oran
*Naval Research Laboratory, Washington, DC*

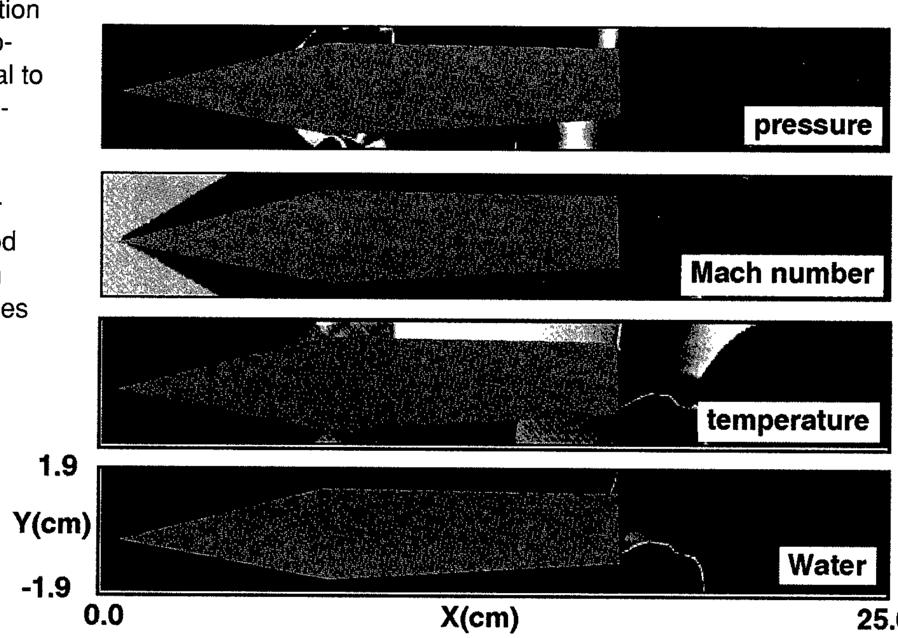
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To study projectile stability, which is crucial to ram accelerator development. The ram accelerator is a propulsion concept based on using shock-induced combustion to accelerate projectiles to very high velocities.

***Methodology:*** Numerical simulations are used to provide pressure distributions on projectiles, slightly perturbed in position, to determine if the perturbation is augmented or corrected by the pressure imbalance on the projectile body. In these simulations, the conservation equations for mass, momentum, energy, and individual species are solved using the flux-corrected transport algorithm (FCT) in conjunction with a two-step, reduced-chemistry model. The virtual cell embedding (VEC) technique is used to accurately represent the complex shape of the ram-accelerator projectile on an orthogonal mesh.

***Results:*** The simulations performed in this study provide information on the pressure distribution on the projectile. These data are needed to calculate aerodynamic torque generated by the pressure imbalance due to a perturbation in the projectile position. Results show that the aerodynamic torque stabilizes the projectile if the center of mass of the projectile is near the projectile tip, and destabilizes the projectile if the center of mass is close to the projectile base. For the projectile with its center of mass located in the middle part of projectile, the aerodynamic torque stabilizes the projectile if a normal shock is maintained on the rear part of the projectile by the thermally choked combustion and destabilizes the projectile if this normal shock is absent. Because this normal shock is the key element in providing forward thrust on a projectile in a successful launch, projectile canting could be more serious in a failed launch process in which no normal shocks are maintained on the rear part of the projectile.

***Significance:*** The information on the projectile stability obtained in this study is crucial to projectile design in the ram-accelerator development program, supported by the Army, the Navy, and the Air Force. The research method developed in this study can also be applied to other types of propulsion devices.




*Pressure, Mach number, temperature, and water concentration from the simulation of the reactive flow around a ram-accelerator projectile whose axis is rotated 1.5 degrees counterclockwise from that of the launch tube. The normal shock on the upper surface of the projectile is significantly stronger and more forward than that on the lower surface.*

# Magnetic Fluxtube Tunnelling

R.B. Dahlburg, S.K. Antiochos, and D. Norton
*Naval Research Laboratory, Washington, DC*

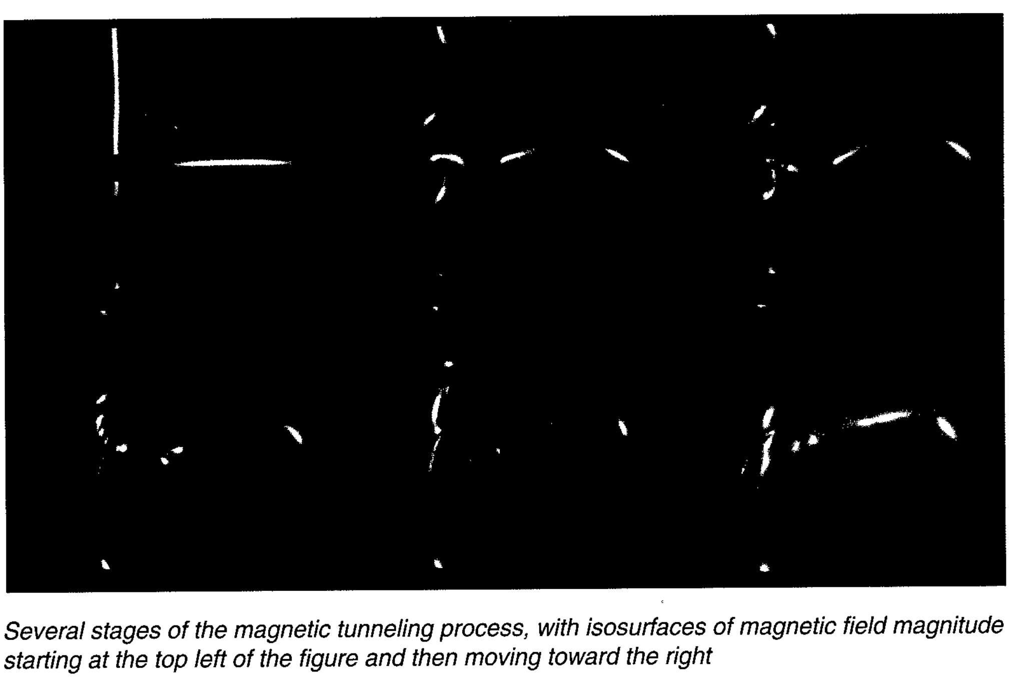
***Computer Resources:*** TMC CM-5E [NRL DC]

***Research Objectives:*** To understand the origin of the fine-scale temporal variability of hard X-ray emission observed in two-ribbon solar flares.

***Methodology:*** It has been hypothesized that the fine-scale temporal structure observed in two-ribbon solar flares is due to the collision and subsequent reconnection of a multitude of magnetic fluxtubes. We model the interaction of two representative uniform twist, force free fluxtubes initially placed orthogonally with respect to each other. The numerical investigation of this process relies on CRUNCH, our highly parallelized explicit Fourier collocation, three-dimensional, compressible magnetohydrodynamics code. This year we have optimized the performance of the CRUNCH code on the NRL CM-5E so that a typical production run with this code at a resolution of $128^3$ Fourier modes requires about 10 hours.

***Results:*** We identified three interactions between initially orthogonal fluxtubes: elastic collision; total reconnection; and the startling case of fluxtube tunneling. The tunneling behavior had not been seen previously in studies of either vortex tube or magnetic fluxtube reconnection. This result arose unexpectedly when the resolution of the fluxtube reconnection simulations was made large enough. The possibility of the occurrence of tunnelling is usually dismissed as a consequence of ideal magnetohydrodynamic theory. Two conditions must be met for tunneling to occur: the magnetic field must be highly twisted, and the Lundquist number must be large. An examination of magnetic field lines shows that tunneling is due to a double reconnection process, by which initially orthogonal magnetic field lines reconnect at two locations, exchange interacting sections, and then pass through each other.

***Significance:*** Reconnection between magnetic fluxtubes has been proposed as the cause of the fine-scale temporal variability of hard X-ray and microwave emission observed in two-ribbon solar flares, a major impediment to communications and space operations. The timescales we observe in our simulations for these interactions are close to those of the observed fine-scale temporal structure in two-ribbon flare hard X-rays. In addition, the discovery of fluxtube tunneling indicates that conventional wisdom has been completely wrong about the number of possible fluxtube interactions.



*Several stages of the magnetic tunneling process, with isosurfaces of magnetic field magnitude starting at the top left of the figure and then moving toward the right*

# Shock Wave Interactions on Double Wedges

M.J. Wright, J. Olejniczak, and G.V. Candler
*ARL/Army High Performance Computing Research Center, Minneapolis, MN*

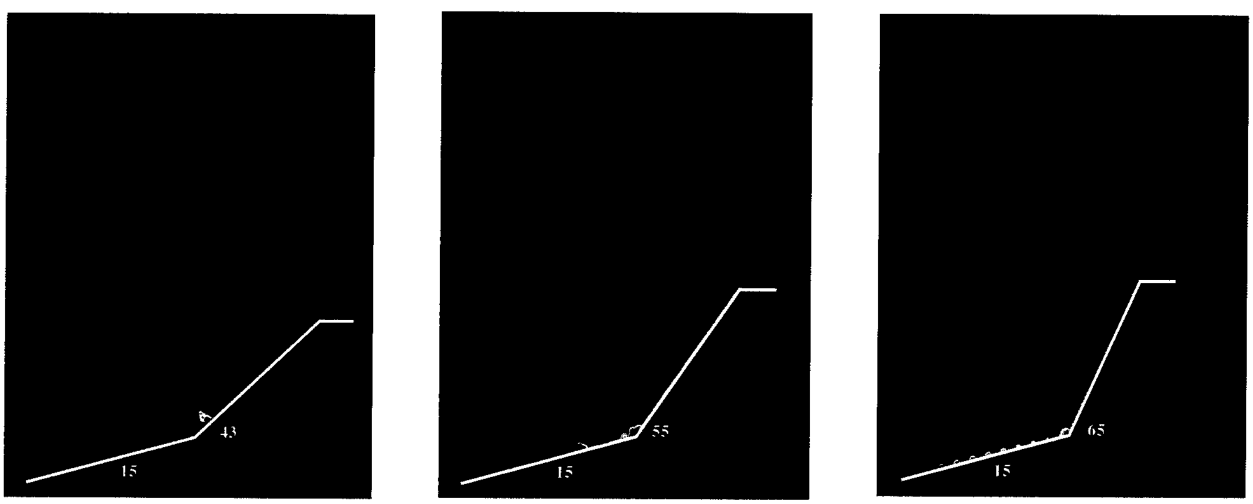
***Computer Resource:*** TMC CM-5 [AHPCRC DC]

***Research Objective:*** To study supersonic flows over double-wedge geometries by using computational fluid dynamics. Under certain conditions, very large local pressure and heat transfer peaks occur, but the mechanism for their formation is poorly understood. These anomalous flow features could affect control surface performance on future high-speed aircraft and missiles.

***Methodology:*** The recently developed Data-Parallel Lower-Upper Relaxation method for solving two- and three-dimensional Euler and Navier-Stokes equations has been implemented on the CM-5. Higher-order upwind differencing methods are used in the implicit, finite-volume formulation. Extremely fine grids (typically 1 million points) are used to resolve the complicated shock interaction process. The method runs at more than 20 Gflops on a 512-node partition of the AHPCRC CM-5.

***Results:*** The calculations have led to a new understanding of how shock interactions occur on double-wedge geometries. The interactions had been classified according to the method of Edney, but a new interaction was found that does not fit the Edney classification scheme. This interaction results in a supersonic jet flowing near the surface of the body, with extremely strong pressure oscillations occurring on the body surface.

***Significance:*** The new computational fluid dynamics method makes it possible to study flow fields in more detail than previously possible. The current work has led to a new understanding of shock interactions on double-wedge geometries, and it has shown that a previously unknown shock interaction may cause very large pressure and heat transfer oscillations on control surfaces of supersonic vehicles.




*Pressure contours in the flow field of three double-wedge geometries in a Mach 6 flow (from left to right). Three different interactions are shown: Edney's Type V (left), Type IV (center), and the new interaction (right).*

# Two-Dimensional Vortex Interaction

J.F. Garten, D.C. Fritts, S. Arendt, and O. Andreassen
*University of Colorado, Boulder, CO*
*Air Force Office of Scientific Research, Washington, DC*

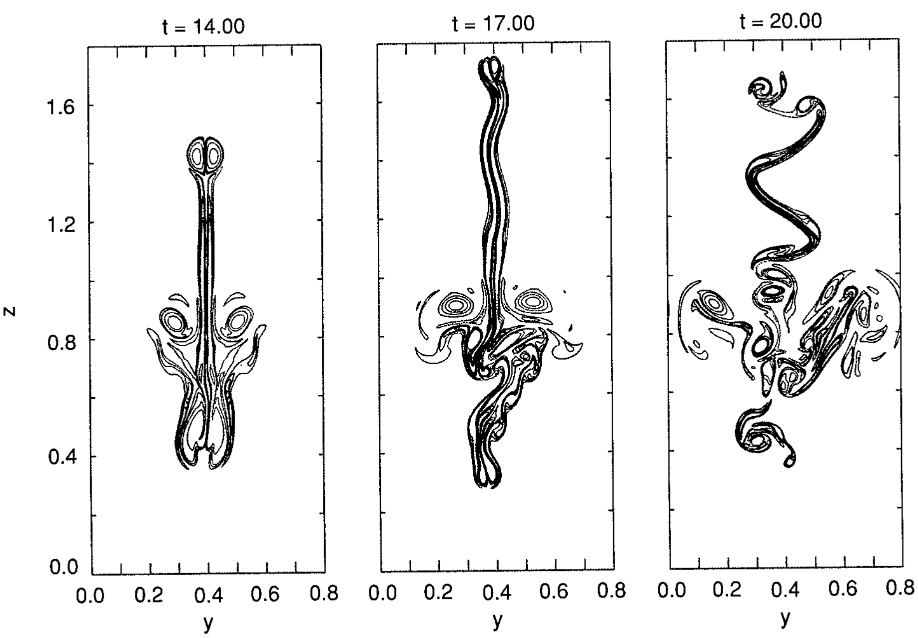
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC and CEWES MSRC]

***Research Objective:*** To investigate the interactions of counter-rotating pairs of vortices by using numerical simulations. The basic theory of the reconnection of trailing vortices behind an airplane wing has been well understood for more than 20 years. Until recently, however, numerical investigations of this problem have generally consisted of parameter space searches, while quantitative understanding of the underlying physical processes has been somewhat neglected. We have formulated our numerical simulations to specifically improve understanding of these previously neglected processes.

***Methodology:*** We have used a four-domain spectral code to solve the Euler equations in a stratified atmosphere subject to compressible and dissipative effects. Fourier functions and periodic boundary conditions were used in the horizontal directions, while Chebyshev functions and open boundary conditions were used in the vertical direction. We specified the initial conditions of two counter-rotating vortices, and the code advanced the flow in time with an explicit time-stepping scheme.

***Results:*** The high-resolution simulations we have run have allowed us to begin broad searches of parameter space. They have also provided detailed quantitative information that has led to useful physical insights into the dynamics. Having examined the two-dimensional simulations already performed and building up a physical understanding of the two-dimensional processes involved in the interaction of two vortices, we have now begun three-dimensional simulations that should quickly add to our understanding of vortex reconnection.

***Significance:*** The analysis of these numerical investigations affects our understanding of airplane safety, specifically, how far apart airplanes should be spaced so as not to encounter coherent vortex structures left behind by other airplanes.




*Contours of positive (red) and negative (blue) vorticity are shown at times t = 14, 17, and 20 in nondimensional time units. The high spatial resolution allows confident examination of the asymmetries that appear at late times in the evolution.*

# Direct Numerical Simulation for the Receptivity and the Whole Process of Transition Around 2-D Airfoils

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*Louisiana Technical University, Ruston, LA*
*Air Force Office of Scientific Research, Washington, DC*

***Computer Resource:*** Cray C916 [NAVOCEANO MSRC] and IBM SP2 [MHPCC DC]

**Research Objective:** To develop a very accurate and very efficient multigrid direct numerical simulation (DNS) code to simulate the real time-dependent compressible turbulent flow around Air Force flight vehicles without using turbulence models.

***Methodology:*** The DNS codes, including grid generation, base flow, and perturbation flow codes, have been developed and are being used to investigate the whole process of flow transition in the two-dimensional (Joukowsky) airfoil boundary layers. The numerical investigation is based on the so-called spatial approach. A contravariant-based governing system is derived so that we can simulate the receptivity and transition around complex geometric configurations.

***Results:*** Simulations have been made on several configurations. Numerical results agree very well with experimental results for the flat plate case, and also agree very well with the results obtained for the 2-D ellipse-leading edge receptivity case. For the airfoil cases, we found the rate of receptivity to be much weaker than the ellipse-leading edge case, but the amplification rate to be much stronger and easier to break down.

***Significance:*** Direct numerical simulation for the entire process of transition around relatively complex geometry is now available by using supercomputers and the approach we have developed. In the near future we expect to be able to do more realistic problems and simulate the real time-dependent compressible turbulent flow around Air Force flight vehicles without using turbulence models.


*Instantaneous contour plots of perturbation $w_z$ on the $j = 6$ ($\approx 0.07h$ from wall) grid surface at $t = 17T$. $Re_L = 200{,}000$ ($Re_h = 5000$), $F = 200$, chordlength/half-thickness = 40; grids: $402 \times 32 \times 26$*

# Three-Dimensional Separation in a Supersonic Cylinder-Flare Turbulent Interaction

D.V. Gaitonde and J.S. Shang
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

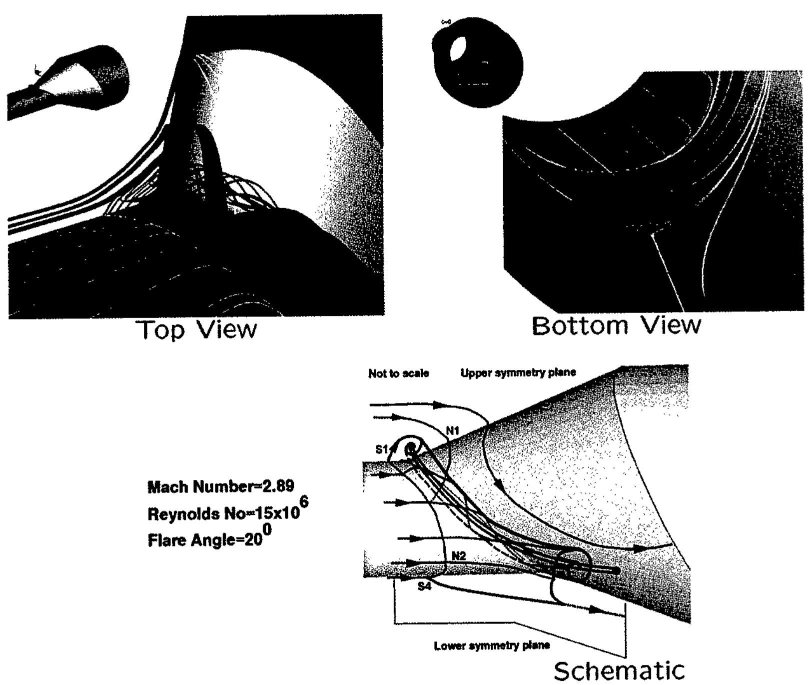
***Computer Resource:*** Cray C916 [CEWES MSRC and NAVOCEANO MSRC]

***Research Objectives:*** To examine the three-dimensional external shock wave/turbulent boundary layer interaction caused by a cylinder/offset-flare juncture at Mach 3. The emphasis of this study is twofold: to examine the accuracy of a hierarchy of zero-, one-, and two-equation turbulence models in engineering prediction; and to analyze the flowfield from a topological perspective.

***Methodology:*** The mean compressible full Navier-Stokes equations are solved with high-resolution upwind methods. Turbulence closure is achieved with the Baldwin-Lomax algebraic model, the two one-equation procedures of Baldwin-Barth and Spalart-Allmaras, respectively, and a variant of the two-equation $k$-$\varepsilon$ model.

***Results:*** Comparison with experimental data reveals that, with minor variations, all models successfully reproduce most flow features, including the inviscid shock, upstream influence and surface pressures. Deviations in skin friction coefficient are analyzed. The dominant aspects of the surface topological portrait are successfully predicted. The flow structure is relatively insensitive to turbulence model and exhibits several of the complex features associated with 3-D separation. The principal feature is a horseshoe-like vortical structure whose legs wrap around the juncture and are turned streamwise near the lower symmetry plane.

***Significance:*** Shock-wave turbulent boundary layer interactions are ubiquitous in supersonic aircraft components. The methods evaluated show that despite the complexity of turbulence, adequate predictions can be obtained of mechanical and thermal loading to assist in efficient design against catastrophic failure. Flow separation in three dimensions is fundamentally different from that in two-dimensional situations. A clear understanding of the process as presented here is a starting point for the development of efficient flow control techniques to reduce performance degradation caused by separation.




*Vortical flow field of supersonic cylinder/offset flare juncture*

# Instabilities in the Shear Layer of Delta Wings

R.E. Gordnier and M.R. Visbal
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

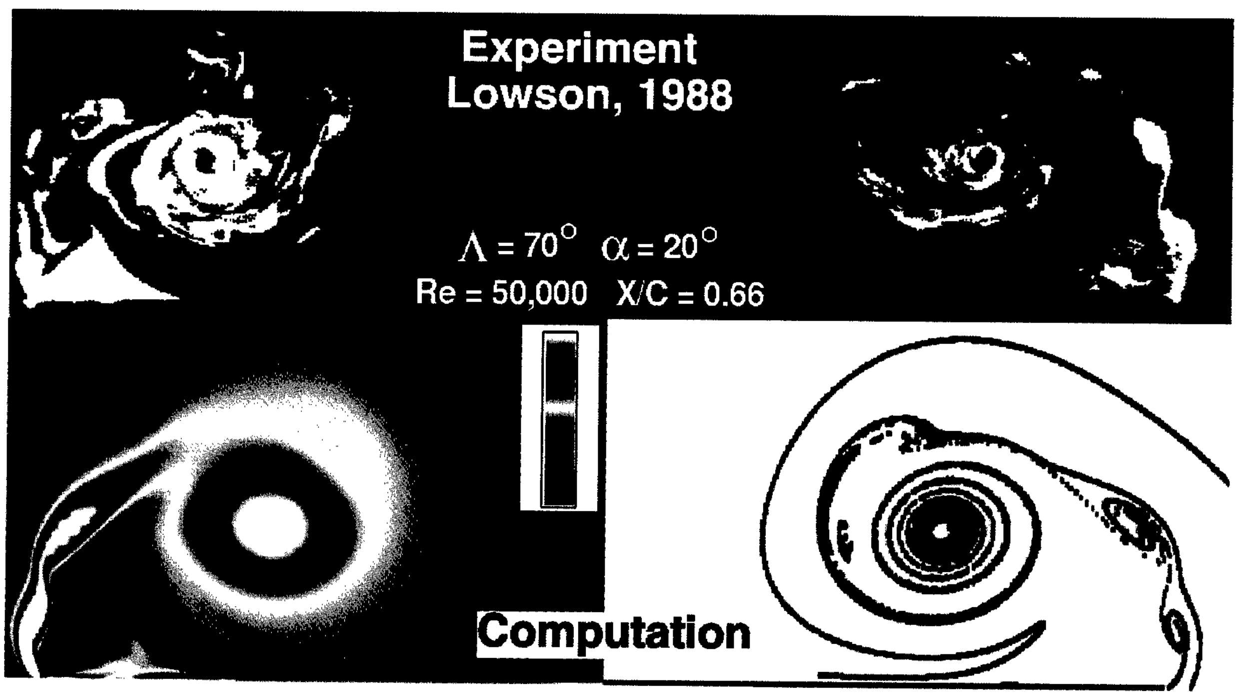
***Computer Resource:*** Cray 916 [CEWES MSRC and NAVOCEANO MSRC]

***Research Objective:*** To numerically simulate and investigate unsteady, vortical substructures observed in the shear layer flowing from the leading edge of delta wings.

***Methodology:*** The unsteady, three-dimensional (3-D), full Navier-Stokes equations are solved by using the implicit, approximately factored Beam-Warming algorithm. The resulting flow code has been fully vectorized and optimized for efficient operation on large vector processing machines.

***Results:*** Unsteady, 3-D, vortical structures observed in the shear layer flowing from the leading edge of delta wings have been simulated numerically. The computed shear-layer unsteadiness and roll-up have been shown to be closely linked to the boundary-layer eruptive behavior induced by the vortex/surface interaction. Reynolds number, sweep angle, and angle of attack were all seen to influence the shear-layer unsteadiness. The variation of the shedding frequency along the leading edge was found to become increasingly linear as the shear-layer instability is amplified.

***Significance:*** The present results provide insight into the basic mechanisms for vortex formation over aircraft and missiles at high angle of attack. They also lead to an improved understanding of experimental flow visualizations. Enhanced understanding of the shear-layer structure has direct bearing on vortex and shear-layer control techniques used to manipulate vortices over aircraft at all angles of attack.




*Comparison of simulated shear-layer vortical structures with experiment*

# 3-D Shock Wave/Turbulent Boundary Layer Interaction Using a Full Reynolds Stress Equation Model of Turbulence

D.D. Knight and G. Zha
*Rutgers University, New Brunswick, NJ*
*Air Force Office of Scientific Research, Washington, DC*

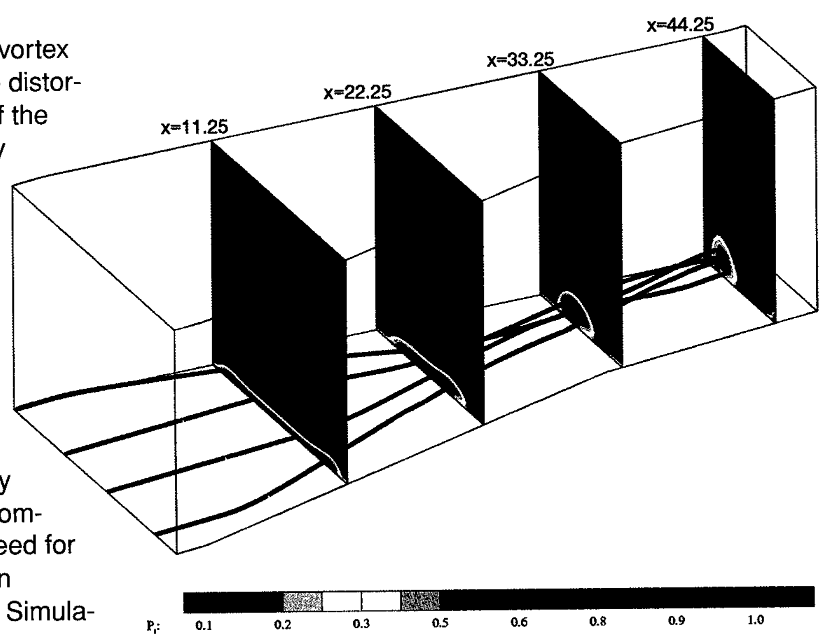
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC and CEWES MSRC]

***Research Objectives:*** To evaluate the capability of a full Reynolds stress equation (RSE) turbulence model to predict the flowfield in a strongly three-dimensional (3-D) shock-wave turbulent boundary layer interaction by comparison with experiment, and to analyze the flowfield structure.

***Methodology:*** The full 3-D compressible Reynolds-averaged Navier-Stokes equations are solved using a full Reynolds stress equation (RSE) model of turbulence. The numerical algorithm uses Roe's flux difference splitting for the inviscid terms, central differencing for the diffusion and source terms, and Euler implicit differencing in time. A series of computations with different grids was performed to establish the accuracy of the numerical simulations.

***Results:*** Computations have been performed for the 3-D shock-wave turbulent boundary layer interaction generated by an asymmetric crossing shock interaction. The crossing shocks are created by 7- and 11-degree fins affixed normal to a flat plate. The freestream Mach number is 3.85, and the Reynolds number based on the upstream boundary layer thickness is 0.30 million. Experimental data include surface pressure, surface flow visualization, adiabatic wall temperature, and heat transfer. The computed surface pressure agrees closely with experiment. The adiabatic surface temperature is predicted within 5 percent. The heat transfer coefficient overestimates the peak experimental value by 80 percent within the 3-D interaction, pointing to an obvious need for the development of Large Eddy simulation methodologies with improved turbulence models, which are capable of predicting turbulence structure and its evolution in complex flows. The simulations show that the principal streamline feature is an asymmetric counter-rotating vortex pair, generated by the initial oblique shock wave-turbulent boundary layer interactions, which is responsible for the significant total pressure distortion downstream of the interaction. The figure shows these effects and displays streamlines and the total pressure normalized by the upstream freestream total pressure.

***Significance:*** The counter-rotating vortex pair is principally responsible for the distortion observed in high-speed inlets of the sidewall compression type, and may serve as an efficient mixing mechanism for an integrated scramjet inlet-combustor. This would improve combustion efficiency, thus reducing drag and engine size and improving aircraft performance. The inability of a full RSE turbulence model to predict accurately the surface heat transfer has been proven and emphasizes the difficulty of accurate simulation of complex compressible turbulent flows, and the need for more accurate turbulence simulation methodologies such as Large Eddy Simulation incorporating improved turbulence modeling.




*Streamlines and relative total pressure contours for crossing shock wave-turbulent boundary layer interaction*

# Large-Eddy Simulation of Flow Around an Airfoil

P. Moin and K.E. Jansen
*Stanford University, Stanford, CA*
*Air Force Office of Scientific Research, Washington, DC*

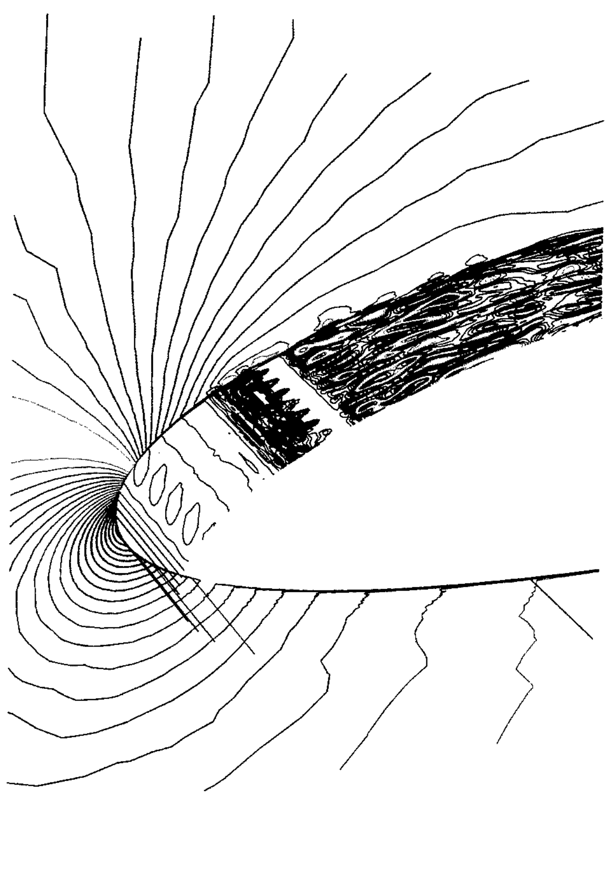
***Computer Resource:*** TMC CM-5 [AHPCRC DC] and TMC CM-5E [NRL DC]

***Research Objective:*** This work represents a fundamental advance in large-eddy simulation (LES) technology. Unstructured meshes will allow not only complex geometries to be discretized but will also allow cost-efficient resolution of near-wall features. Resolution of these scales has in the past limited LES to fairly low Reynolds numbers. By refining the unstructured grid only where necessary, a much higher Reynolds number may be obtained for the same number of nodes.

***Methodology:*** The three-dimensional (3-D) compressible Navier-Stokes equations are solved on an unstructured mesh via a Galerkin/least-squares finite-element method. This method has been shown to be quite efficient on the CM-5, where the algorithm averages 25 Mflops per processing node. This results in an equivalent flop rate of 30 Cray C90 single processors. The subgrid scale model used a variant of the dynamic model. This model requires filtering of the velocity field to determine the subgrid scale viscosity. Filters have been developed for the unstructured grid and have been shown to be both effective and efficient.

***Results:*** Preliminary results are presented for the LES of an NACA 4412 airfoil at maximum lift and a Reynolds number of 1.64 million. Before we can compare the results to the experiment, we must represent the transition strip used in the experiment. The unstructured grid allows discretization of the serrated tape. The figure shows the laminar flow before, and the turbulent flow after the transition strip.

***Significance:*** The flow described is representative of many flows that are not well predicted by current techniques used in industry (Reynolds-averaged Navier-Stokes). With further research, LES using unstructured grids will meet the challenge of this and other difficult flows in an efficient manner.



*Streamwise velocity contours on two planes of the 3-D flow—the airfoil cross-sectional plane and a plane parallel to the airfoil surface inside the turbulent boundary layer, cutting through the serrated transition strip (high-speed fluid, red; low-speed fluid, blue)*

# Large-Eddy Simulations of Ship Wakes

D.G. Dommermuth
*Science Applications International Corporation, San Diego, CA*
*Office of Naval Research, Arlington, VA*

***Computer Resource:*** TMC CM-5 [AHPCRC DC] and TMC CM-5E [NRL DC]

***Research Objectives:*** To quantify how free-surface turbulence affects the remote sensing of ship wakes and to develop capabilities to understand and model ship wakes. Results of this research will benefit a Department of Defense Ship-Wake Program whose major focus is the detection of ship wakes. The results of the research will also ultimately improve our modeling of turbulent flows in general.

***Methodology:*** The finite-difference method that we have developed for this project has been optimized for performance on CM-5 computers. CM-5 computers are absolutely essential to this research because the numerical simulations of ship wakes, in particular the interaction of turbulence with waves, require large amounts of CPU and memory.

***Results:*** Our research over the past year has focused on modeling turbulence by using large-eddy simulations (LES). Our numerical simulations compare well with model-test experiments of a naval frigate. Prior to our numerical simulations, based on laboratory experiments it had been believed that turbulent free-surface flows would obey two-dimensional scaling laws. However, our numerical simulations show that turbulent roughening of the free-surface scales according to three-dimensional similarity theory. Our numerical results were made possible by the development of a new technique for initializing LES.

***Significance:*** We now have an improved understanding of how ship wakes behave. This understanding leads to the development of new techniques for the remote detection of ships. In addition, our new technique for modeling turbulence has applications in large-eddy simulations and Reynolds-averaged Navier-Stokes simulations.

*Wake of a model-scale frigate; the wake spreads more at the free surface because the free surface acts as a reflection boundary*

# Turbulent Viscous-Inviscid Interactions at Mach-4

D.V. Gaitonde and J.S. Shang
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

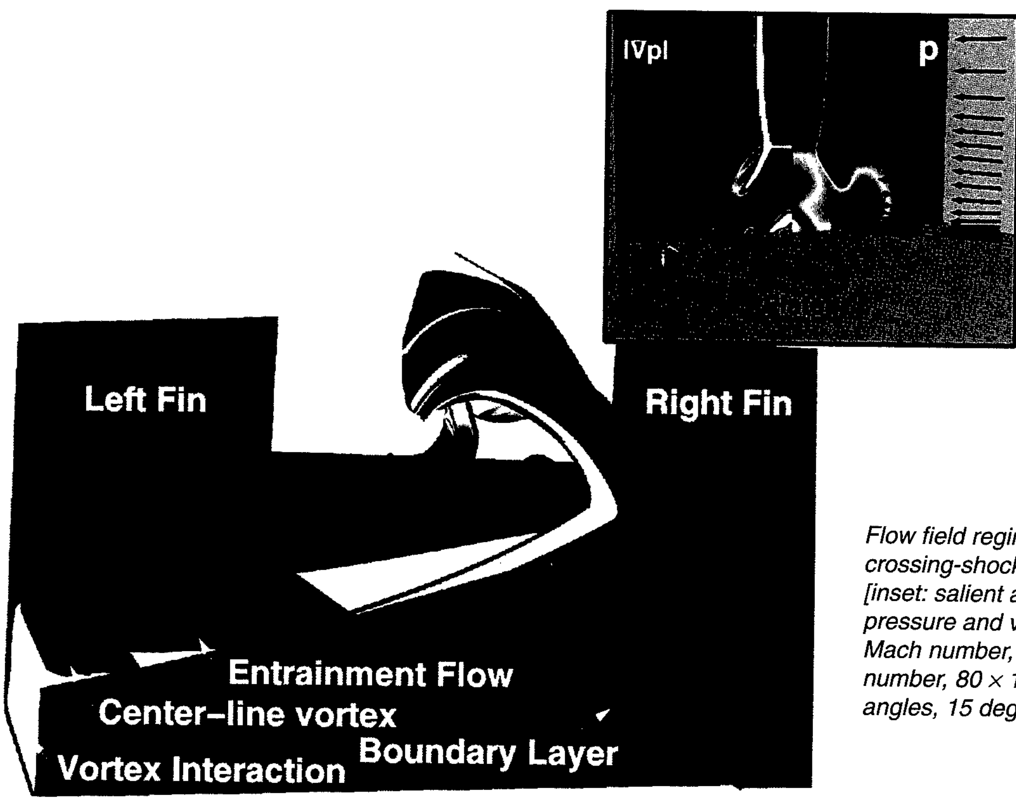
***Computer Resources:*** Cray C916 [CEWES MSRC and NAVOCEANO MSRC]

***Research Objective:*** To examine the viscous-inviscid interaction in a supersonic inlet-type geometry consisting of two fins mounted on a flat plate. Of particular interest is the relationship between the kinematic structure and features of engineering interest, specifically surface shear stresses and heat transfer rates.

***Methodology:*** The full mean compressible Navier-Stokes equations are solved. Turbulence effects are incorporated with several eddy-viscosity-based models of varying complexity. Numerical issues addressing simulation integrity are carefully examined. Post-processing techniques use unique approaches to identify and analyze three-dimensional coherent structures.

***Results:*** Good agreement is obtained with experiment for surface pressure, pitot surveys, shock structure, and surface streamlines. The figure describes the flow in terms of four distinct regimes: separated boundary layer, vortex interaction flow, symmetric centerline vortices, and entrainment flow. The inset frame shows elements of the shock system at a crossflow plane and velocity field development with a prominent wall-jet-like structure near the plate.

***Significance:*** These results have significant implications on supersonic inlet design. In addition to providing reasonable estimates of surface loading, the flowfield structure can also be used to describe the performance of such devices and to improve efficiency. For example, these calculations clearly show that the fluid constituting the centerline vortices originates upstream, from near the leading edges of the fins. Of particular concern is the occurrence of a large separated region of low recovery and the existence of off-surface stagnation points in the flow. This field distortion adversely affects inlet efficiency.




*Flow field regimes in crossing-shock interactions [inset: salient aspects of pressure and velocity fields]. Mach number, 4; Reynolds number, 80 × $10^6$/m; fin angles, 15 degrees.*

# Efficient Parallel Flow Solver

R. Pankajakshan and W.R. Briley
*Mississippi State University, Starkville, MS*
*Office of Naval Research, Arlington, VA*

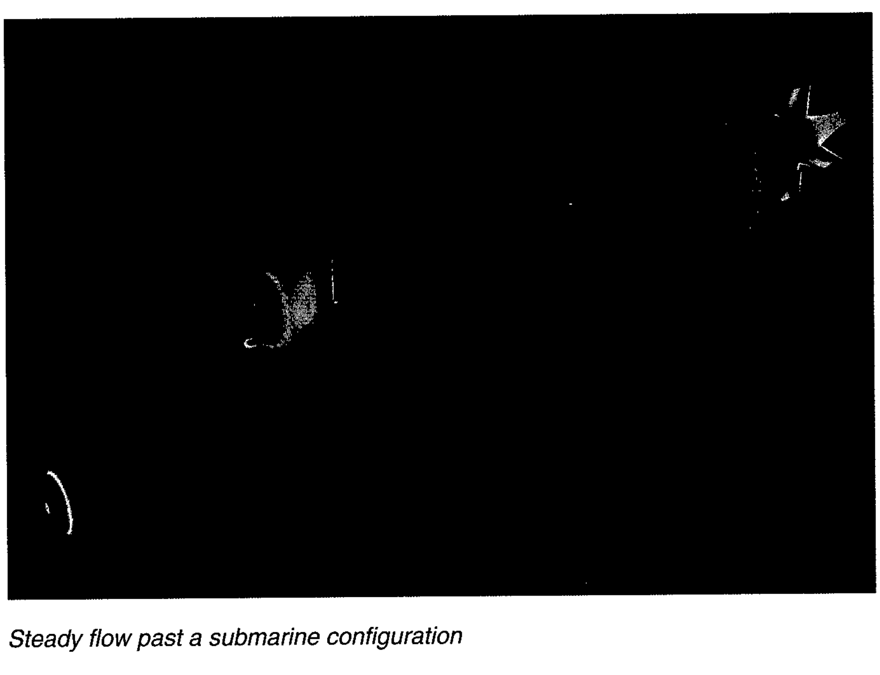
***Computer Resource:*** IBM SP2 [MHPCC DC]

***Research Objective:*** To develop an efficient parallel flow solver for large-scale unsteady viscous incompressible flow simulations on multiblock structured grids. This is part of a larger study of flows around maneuvering undersea vehicles sponsored by the Office of Naval Research.

***Methodology:*** The flow solver uses an artificial compressibility formulation to solve the three-dimensional unsteady incompressible time-averaged Navier-Stokes equations in multiblock transformed coordinates. The parallel implementation uses domain decomposition to partition and map the data space onto a set of processors. Static load balancing is done at the grid-generation stage based on a heuristic performance estimator that takes into account the characteristics of the algorithm and the available system resources. The time-linearized approximations of the governing equations are solved at each time step using a block-decoupled symmetric Gauss-Seidel relaxation procedure. This involves a point-to-point message exchange at each subiteration level. The algebraic turbulence model also includes user-defined collective operations over processor subsets. The code uses MPI because of its extensive portability and functionality.

***Results:*** Steady solutions for a submarine hull with both sail and rear appendages were timed on the IBM RS/6000 SP at MHPCC for cases using 0.6 million points (12 128Mb processors) and 3.3 million points (32 256Mb processors). The 500 time steps for the 0.6M point case required 40 minutes (85 percent CPU, 480 Mflops), and the 3.3M point case would require 80 minutes (81 percent CPU, 1.2 Gflops). For comparison, a fully appended case with body-force propulsor has been run with a sequential multigrid version of the code on a single IBM-590 workstation and required 43 CPU hours (518Mb) for 2.5M points.

***Significance:*** The state-of-art parallel solution of submarine flows is advanced by enabling the computation of large-scale unsteady incompressible flows past fully appended submarine configurations with good efficiency and reasonable run times, with portability across different parallel computing platforms based on MPI, and with demonstration on the IBM RS/6000 SP at MHPCC.



*Steady flow past a submarine configuration*

# Navier-Stokes Simulations on Massively Parallel Supercomputers

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*Lockheed-Martin Skunk Works, Palmdale, CA*
G. Montry
*Southwest Software, Albuquerque, NM*
V. Jackson, A. Bessey, and T. Phung
*Intel Scalable Systems Division, Beaverton, OR*
L.J. Huttsell and E. Turner
*Wright Laboratory, Wright Patterson Air Force Base, OH*

***Computer Resource:*** Intel Paragon [ASC MSRC]

***Research Objective:*** To develop a version of the ENS3D multiple-zone three-dimensional Navier-Stokes flow simulation code, which operates efficiently on the Intel Paragon massively parallel processor (MPP). MPP supercomputer architectures offer the potential for increased speed and memory capacity, with reduced cost per calculation over using traditional vector/parallel supercomputer architectures. The ENS3D code was originally developed for vector/parallel shared-memory supercomputers.

***Methodology:*** A version of the ENS3D code was ported to the distributed memory Intel Paragon MPP. Parallelization on the MPP was obtained by using extensive explicit message-passing. A one-dimensional domain decomposition was used per grid zone. Multizone problems are efficiently solved by mapping each grid zone into a compute partition on the MPP and integrating all grid zones in time concurrently. This allows operation on hundreds or thousands of compute nodes.

***Results:*** Large-scale Navier-Stokes simulations of complete aircraft on grids ranging up to 30 million points have been obtained. The figure shows a typical application for an advanced fighter configuration at Mach 0.17 and 30-degree incidence, with vortex formation off the leading edges of the canards and wings. Timing results are given for simulations with varying number of compute nodes and grid sizes. Cost studies have shown a 75 percent reduction in cost per calculation using the Intel MPP over vector/-parallel supercomputers.

***Significance:*** Large-scale Navier-Stokes simulations can be performed with low-wall-clock execution times and with significantly reduced cost per calculation ratios over using traditional vector supercomputers.

*Fighter configuration showing vortex formation*

Compute times versus grid size and number of compute nodes

| Number of Grid Points | Number of Compute Nodes | Compute Time (hr) |
|---|---|---|
| 3,075,200 | 240 | 2.85 |
| 3,075,200 | 480 | 1.51 |
| 8,323,200 | 800 | 2.46 |
| 21,632,000 | 1024 | 4.82 |
| 29,744,000 | 1024 | 6.94 |

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# Computational Chemistry and Materials Science

*Computational Chemistry and Materials Science focuses on the modeling and design of new chemical compounds, chemical reaction systems, and materials for DoD mission applications. The information gathered from CCM calculations often cannot be obtained from experiments and leads to understanding the important physical, chemical, optical, and mechanical properties required to tailor-make chemical processes and materials for specific applications. The 12 success stories in this section represent the broad spectrum of research covered in CCM—from environmental clean-up and superconducting materials research to research in explosives and rocket propellants. Two major accomplishments in CCM are discussed in the stories on new conducting and semiconducting polymers (page 83) and the development of new aircraft de-icing chemicals (page 84), both designed with CCM calculations.*

Capt. Scott G. Wierschke
Phillips Laboratory
Edwards Air Force Base, CA
CTA Leader for CCM

# Half-Metallic Manganese Oxide Magnets

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*Naval Research Laboratory, Washington, DC*

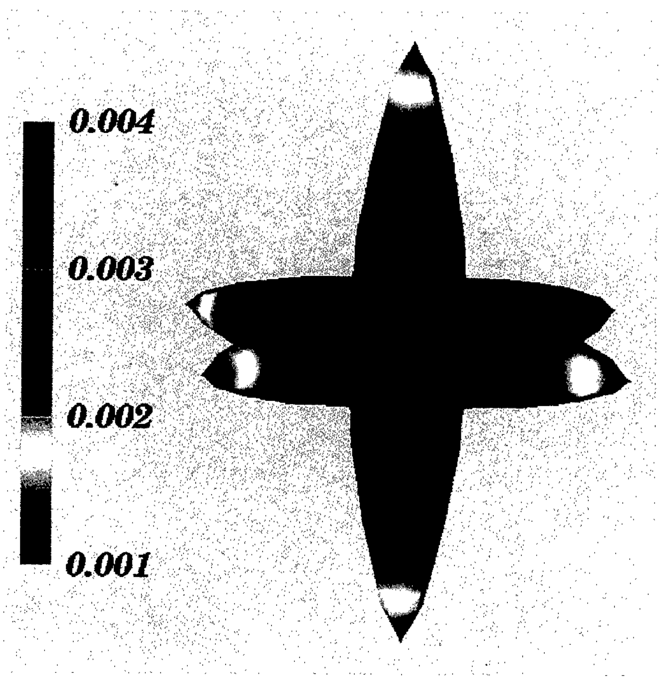
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC]

***Research Objectives:*** To provide a microscopic basis for describing (understanding and predicting) the salient properties of the new class of magnetic alloys now known as "colossal magnetoresistance" (CMR) materials. The alloys show even greater decreases in resistivity due to an applied magnetic field than do the "giant magnetoresistance" systems, hence the term "colossal." The microscopic, quantum mechanically based theory is used to describe the electronic, magnetic, and crystal structures, and finally the transport properties, of magnetic materials of importance to the Navy. The CMR materials are particularly difficult because of a complex interrelationship between structural, electronic, and magnetic behavior.

***Methodology:*** The density functional approach is used to describe the behavior of electrons in a solid. Completely general codes, state of the art in precision, are used. The many-body problem is reduced to the self-consistent solution of coupled, nonlinear second-order differential equations that are solved by a combination of linear algebra techniques and iterative refinements. Many-body effects are currently described by a local density approximation, but extensions of this method are being implemented.

***Results:*** The crystal energies and full electronic structure have been calculated for a variety of magnetic orderings and including effects of structural distortions in the CMR system $La_{1-x}Ca_xMnO_3$. The observed crystal structure and magnetic order was obtained correctly in all cases studied. In the ferromagnetic regime, where the material is metallic, we show that it is effectively "half-metallic," that is, electrons with spin up are metallic while electrons with spin down are insulating. This is a highly unusual occurrence in solids, and must be related to the CMR effect that is also highly unusual (unique, so far).

***Significance:*** This class of CMR materials is envisioned for applications in magnetic field sensors. Specific implementations range from the detection of submerged submarines to magnetoelectronic devices necessary for stable, high-density magnetic recording. The property, already demonstrated, that the temperature of peak magnetoresistance can be tuned by varying the oxygen or cation concentration will be exploited to optimize each specific application.




*Surface in momentum space (Fermi surface) containing the minority spin charge carriers in ferromagnetic (La,Ca)$Mn_3$. Color indicates the carrier velocity, which is small for all carriers.*

# Improved Synthesis of Cubane

E.J. Wucherer
*Phillips Laboratory, Edwards Air Force Base, CA*

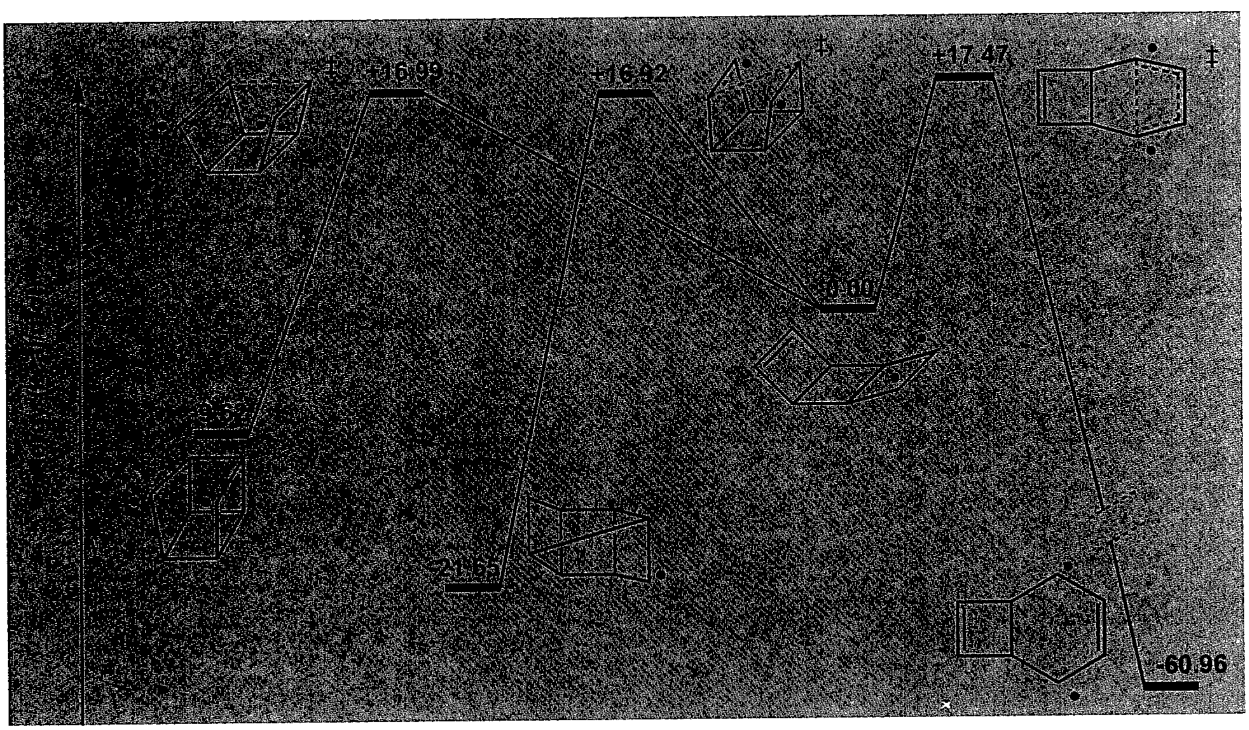
***Computer Resource:*** IBM SP2 [MHPCC DC] and Cray C916 [CEWES MSRC]

***Research Objective:*** To discover if cubane can be prepared from tricyclo[4.2.0.0.]octa-3,5-diene by examining the triplet potential energy surface for C8H8 hydrocarbons and to determine the perturbations to the system that favor the preparation of cubane.

***Methodology:*** Use state-of-the-art ab initio quantum mechanics calculations to model accurately (using the program package GAMESS) the energetics of the bonding geometries expected for the starting materials, products, and transition states. Include configuration interaction and multiconfiguration self-consistent field methods to account properly for mixing of electronic configurations in the gas phase species. When a consistent energy description is achieved, proceed to calculations in the presence of a reaction field to attempt to model condensed phase effects that should be present in a reaction solution (solvent effect).

***Results:*** Thus far, geometries of four energy minima and three transition states have been optimized at the UHF/6-31++G(d,p) level and further characterized by UMP2 single-point calculations. This interim result indicates that, contrary to published reports, the cubane product should be accessible from the tricyclic starting material. The final energy relationships are likely to change as we progress to correlated methods, so the interim result is interesting but also is to be regarded with suspicion.

***Significance:*** Production of cubane from tricyclo[4.2.0.0.]octa-3,5-diene would represent a substantial reduction in the synthetic pathway, from eight down to two steps. This improvement would greatly facilitate work examining cubane as an ingredient in energetic materials and propellants.




*UMP2/6-31++G(d,p)//UHF/6-31++G(d,p) relative energies of triplet C8H8s*

# A New Stable Surface of Silicon: Si(5,5,12)

S.C. Erwin, A.A. Baski, and L.J. Whitman
*Naval Research Laboratory, Washington, DC*

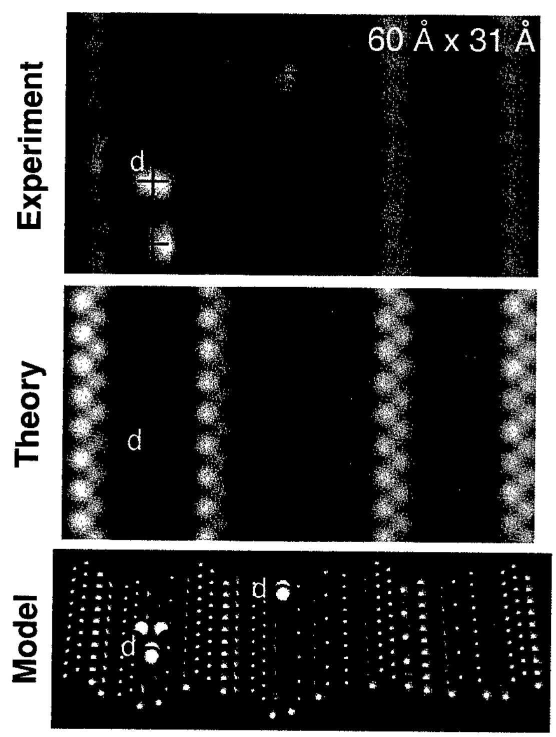
***Computer Resource:*** IBM SP2 [MHPCC DC]

***Research Objective:*** To elucidate the structure of a newly discovered stable surface of silicon known as Si(5,5,12). We use first-principles theoretical methods to predict what a scanning tunneling microscope (STM) would see at this surface, and then compare the predictions to our own actual STM images.

***Methodology:*** We began with an approximate idea, based on our STM images, of the surface atomic structure. We then used state-of-the-art methods to calculate theoretically the quantum-mechanical wave functions at the surface. This simulates what the STM probes experimentally. Our method is density-functional theory in the local-density approximation (LDA). This particular implementation of LDA, developed over the past five years at NRL and elsewhere, is particularly well suited to very large systems such as the Si(5,5,12) surface.

***Results:*** The agreement between our experimental and theoretical STM images is extraordinary, and essentially confirms—in both large-scale and detailed features—our proposed structural model for this remarkable new surface (see figure). Further studies are now in progress to analyze the role of compensated strain in this surface. Coupled with our ongoing experimental work, this research will lead to a better understanding of what makes certain high-index surfaces stable.

***Significance:*** Modern microelectronics are typically fabricated on a silicon substrate whose surface is aligned with the axes of the underlying crystal. These surfaces, called "low-index," are easily prepared and very stable. Researchers now are considering using "high-index" stepped surfaces as substrates for specialized applications. Until now, only one such high-index silicon surface has been known to be stable. We have shown experimentally that Si(5,5,12) is another stable high-index surface. We then used theoretical and computational methods to establish and verify a detailed picture of the microscopic surface structure of Si(5,5,12). As the basis for a multibillion-dollar microelectronics industry, silicon will continue in this role well into the next century. The next generation of advanced technologies will depend on our ability to manipulate this extraordinary material in new ways. For applications such as heteroepitaxy and the growth of one-dimensional structures, rapid progress hinges on understanding the underlying substrate. Our characterization of the Si(5,5,12) surface demonstrates how the structure of even a complicated semiconductor surface can be understood in great detail, given the right experimental and theoretical tools.




*Experimental and theoretical STM images of the Si(5,5,12) surface, based on the structural model, show excellent agreement (crosses indicate adsorbed silicon dimers "d", which occur naturally in the model)*

# Conducting and Semiconducting Polymers by Design

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X.F. Duan and A.T. Yeates
*Wright Laboratory, Wright-Patterson Air Force Base, Dayton, OH*
J.H. Weare
*University of California San Diego, La Jolla, CA*
*Office of Naval Research, Arlington, VA*
*Air Force Office of Scientific Research, Washington, DC*

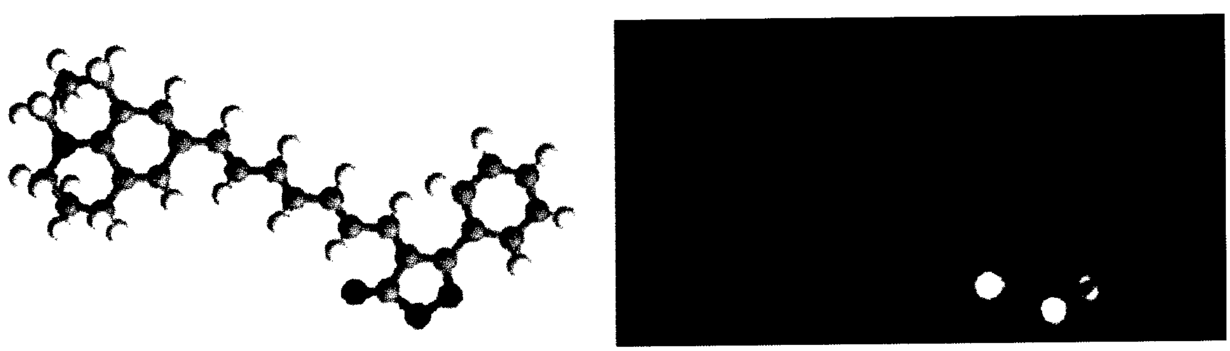
***Computer Resource:*** TMC CM-5 [NRL DC and AHPCRC MSRC]

***Research Objective:*** To predict reliably chemical and physical properties of conjugated polymers and to design new electronic and optical materials based on these molecules. Conjugated polymers provide a new class of conducting and optical materials. To achieve these goals, highly efficient first-principles calculation codes must be developed for massively parallel computers and networks of workstations.

***Methodology:*** The atomic geometry and electronic properties are computed by using the local spin density function method. A planewave basis set is used to capture properties of the delocalized conduction electrons. For large systems, more than 100,000 basis functions per orbital are needed. However, the cost of this large number of basis functions is offset by high parallelism of the algorithms. Our new parallel ab initio molecular dynamics (PAIMD) simulation code allows us to simulate large polymer systems efficiently on the TMC CM-5. The code scales perfectly up to 256 processors.

***Results:*** The magnitude of dimerization plays an important role in semiconducting conjugate polymers, especially for narrowband gap systems. We have optimized the geometry of many p-conjugated carbon systems using oligomers, rings, and infinitely long chains. With optimized oligomers, we have estimated the accurate energy gap by calculating single-triple excitation energy.

***Significance:*** The development of ab initio electronic structure calculation codes for massively parallel platforms using new algorithms is essential for the design of new electronic and optical materials with high performance applications. Our new code is sufficiently accurate and efficient, even for large molecules, that it can be used to expedite material design.



*Structure and electron density of a push-pull polyene calculated by using PAIMD on the TMC CM-5*

# Design of Nontoxic Anti-Icing Compounds

S. Trohalaki and R. Pachter
*Wright Laboratory, Wright-Patterson AFB, OH*

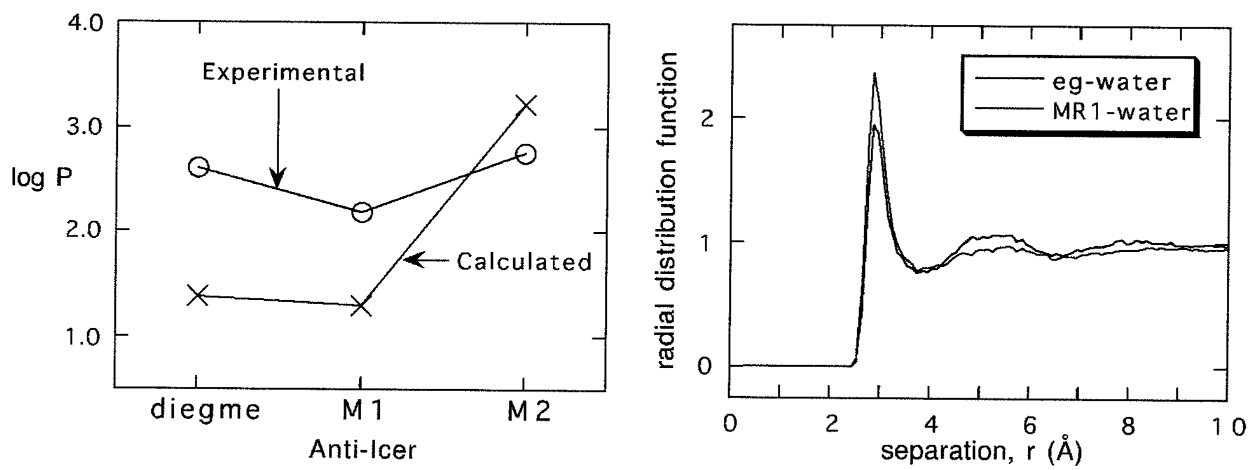
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC and CEWES MSRC]

***Research Objective:*** To design new, nontoxic anti-icing compounds for jet fuel, aircraft wings, and runways by calculating pertinent physical properties and to gain fundamental knowledge of de-icing mechanisms.

***Methodology:*** The calculations used semi-empirical molecular-orbital methods encoded in AMSOL, including solvent effects, and extensive molecular dynamics simulations.

***Results:*** The log of the hexadecane-water partition coefficient, log P, is related to the solvation free energy in water to that in hexadecane, and is an approximation of the partitioning of the candidate molecule between fuel and the water "bottom" typically present in fuel tanks. Partition coefficients in the octanol-water system are extensively applied, also in toxicological predictions. We found that inclusion of the anti-icing compound's geometry response and electronic structure response to the solvent systematically lowers the calculated log P values, thus providing an important predictive capability. It is encouraging that the trends are well reproduced in a comparison of calculated and experimental log P. Molecular dynamics simulations of mixed and de-mixed bulk systems of water and anti-icer permit the extent of hydrogen-bonding to be determined. A comparison to similar analyses of de-mixed systems yields a novel methodology that allows ranking compounds according to their anti-icing performance. Examination of the hydrogen bonding between water molecules with the addition of 50% wt-% ethylene glycol or the same wt-% of candidate anti-icers enabled their effectiveness to be assessed and guided synthesis efforts.

***Significance:*** Anti-icing compounds currently used by the Air Force and Navy in jet fuels dissolve in the water "bottoms" that are present in storage tanks. Hazardous waste, requiring expensive disposal, is thereby produced. Military and civilian airports also use large quantities of toxic runway and wing de-icers; containment is expensive and largely unsuccessful. The development of new, nontoxic anti-icing compounds for jet fuel and de-icing compounds for aircraft wings and runways will thus impact both DoD and civilian requirements.




*Comparison of calculated to experimental log P values (left); intermolecular radial distribution functions for hydroxyl oxygens in ethylene glycol—water and a candidate M1-water mixtures.*

# Shock and Detonation

B.M. Rice, W. Mattson, J. Grosh, and S.F. Trevino
*Army Research Laboratory, Aberdeen Proving Ground, MD*

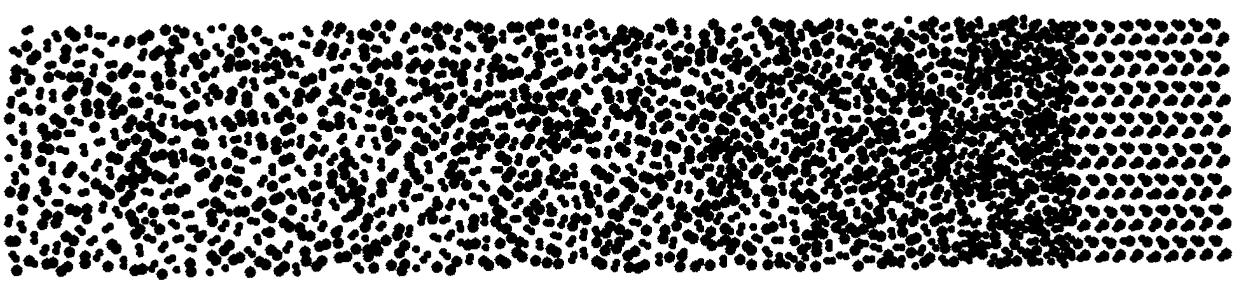
***Computer Resource:*** SGI Power Challenge Array [ARL MSRC]

***Research Objective:*** To provide the first comparison of results from a molecular dynamics simulation of a detonation with hydrodynamic predictions. Also, to determine the reaction mechanism for initiation and sustenance of the detonation.

***Methodology:*** Molecular dynamics simulations, based on classical mechanical equations of motion, are used to calculate the equation of state for this crystal. This, in turn, is used to evaluate the classical conservation equations used in hydrodynamic predictions of detonation. Macroscopic properties of the material behind the detonation wave measured from molecular dynamics simulations of the crystal model subjected to flyer-plate impact are then compared with the hydrodynamic predictions. Because of the enormous CPU requirements for these simulations, new many-body molecular dynamics algorithms were developed for multiprocessing on the ARL MSRC SGI Power Challenge Array.

***Results:*** The Chapman-Jouguet condition for the crystal was determined and compared with the properties behind the detonation wave measured from the computer experiments. Agreement between hydrodynamic predictions and the results of molecular dynamics computer experiments was excellent. Measured detonation wave velocities, densities, and pressures behind the shock wave differ by 6, 0.6, and 2.5 percent, respectively, from the hydrodynamic predictions. Also, the reaction mechanism for the detonation was determined to be pressure-induced atomization of the reactants behind the detonation wave. After the pressure wave passes, these atoms subsequently combine with energetically favored product partners, providing the heat release that sustains the detonation.

***Significance:*** Although the phenomenon of detonation has been explored for more than a century, microscopic details of the chemical and physical changes occurring during the detonation cannot be measured because of the small time and length scales over which the event occurs. Measurements are additionally hampered by the enormous energy release during the detonation. Understanding these microscopic details will lead to the ability to exploit and control this energetic event. Our calculations provide the first direct comparison of results from a molecular dynamics computer experiment to predictions from the well-established hydrodynamic theory of detonation. These calculations have also provided the first elucidation of the mechanism of detonation using a realistic chemical model.



*Snapshot of energetic molecular crystal at 7.8 picoseconds after flyer plate impact; sample dimensions are 300 × 50 angstroms*

# Design of Nonlinear Optical Material Systems

Z. Wang, P. Day, and R. Pachter
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

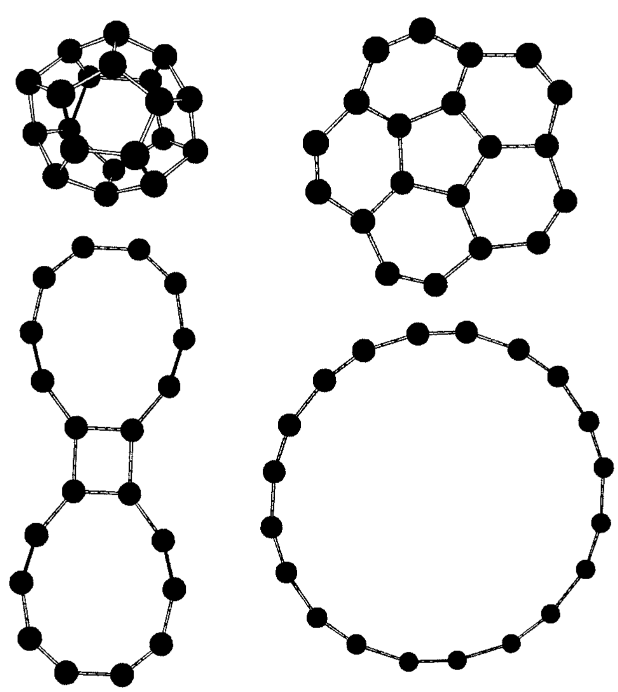
***Computer Resource:*** Intel Paragon [ASC MSRC], Cray C916 [CEWES MSRC], and IBM SP2 [MHPCC DC]

***Research Objective:*** To optimize nonlinear optical (NLO) material and processing properties by reliable calculations of geometries, vibrational frequencies, absorption frequencies, spin-orbit couplings, reaction energetics, polarizabilities, and hyperpolarizabilities of large molecules from first principles.

***Methodology:*** In using Density Functional Theory (DFT) calculations, two functionals of the exchange-correlation energy were used, namely, a Local Density Approximation (LDA), and the gradient-corrected functional of the exchange term by Becke and the correlation term by Lee, Yang, and Parr (BLYP). Hartree-Fock (HF) calculations were carried out with parallel GAMESS.

***Results:*** BLYP geometry optimizations of isomers of $C_{20}$, namely the ring, bowl (corannulene-like), and cage (fullerene-like) configurations, confirm previous single-point calculations based on HF geometries, in favor of the ring geometry, while the LDA results still show a reversed order of energy, favoring the cage geometry. Our calculated LDA vibrational spectra of the ring geometry show significant differences with those of HF in the widths of two band gaps. The Møller-Plesset second-order perturbation theory (MP2) single-point calculations using GAMESS show preference toward the bowl structure, differing from previous similar calculations. The insight gained in modeling $C_{20}$ enables us to make comparative studies with other fullerenes and to assess their relative properties. The stability of pyran has been studied in detail, and has, moreover, shown that infrared spectra are in better agreement with experiment by using DFT rather than HF. The calculations of metallophthalocyanine molecules indicate that these molecules deviate considerably from co-planarity with certain metal substitutions, thus affecting the absorption spectra and important characteristics for optical-limiting requirements and thin-film preparation.

***Significance:*** Reliable properties prediction using first-principle calculations for large molecular systems allow the development of a modeling approach to be used in molecular design studies of novel NLO materials. These material systems are essential for a broad range of DoD applications, including laser hardening.



*The structures of $C_{20}$ isomers: fullerene, bowl, bicyclic ring, and monocyclic ring*

# Computational Chemistry Modeling of Nitric Oxide Formation

D. Bose and G.V. Candler
*ARL/Army High Performance Computing Research Center, Minneapolis, MN*

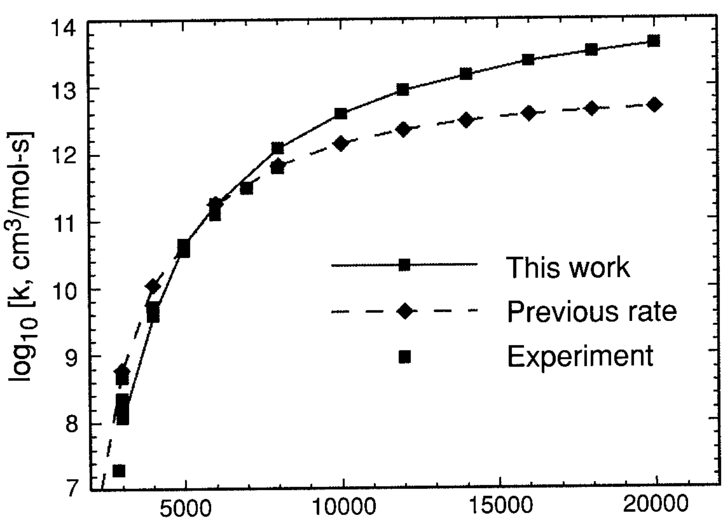
***Computer Resource:*** TMC CM-5 [AHPCRC DC]

***Research Objective:*** To develop an advanced model for the accurate prediction of nitric oxide (NO) formation in reacting flows. This includes hypersonic flow in which there is thermal and chemical nonequilibrium, as well as combustion environments.

***Methodology:*** A parallelized quasiclassical trajectory (QCT) code has been developed and is being used to study the first Zeldovich reaction, $N_2 + O \rightarrow NO + N$, that is the primary mechanism for NO formation in a wide variety of high-temperature flows. The classical equations of motion are integrated on the potential energy surfaces derived from ab initio computational quantum chemistry calculations. The equations are solved using a fourth-order Runge-Kutta scheme in data-parallel on the TMC CM-5. Very large numbers of trajectories (more than a million for low-temperature cases) are computed to get statistically correct results.

***Results:*** The reaction rate of the first Zeldovich reaction has been computed over a wide range of temperatures. Details of the energy disposal during nitric oxide formation have has been studied, and several papers have been published reporting on these results. The figure shows the computed reaction rate of the first Zeldovich reaction, $N_2 + O \rightarrow NO + N$; the computations show that at high temperature the reaction rate is an order of magnitude higher than previously thought.

***Significance:*** Nitric oxide is a major source of pollution in hydrocarbon combustion, and it is a major radiator in re-entry flows. The work has produced the most accurate high-temperature reaction rates for the first Zeldovich reaction, and it has shown that NO is preferentially formed at high vibrational levels. This work will lead to an improved understanding of the details of nitric oxide formation. The reaction rates will make it possible to more accurately predict the amount of NO formed. The quasiclassical trajectory code can be applied to many different chemical reactions so that improved reaction rates can be computed.




*Comparison of the computed reaction rate for $N_2 + O \rightarrow NO + N$ with available data and existing reaction rate expression; computations show that the rate is an order of magnitude larger at high temperatures than previously thought*

# Potential Energy Surfaces for High-Energy $N_2O_2$ Isomers

M.S. Gordon and G. Chaban
*Iowa State University, Ames, IA*
*Air Force Office of Scientific Research, RTP, NC*

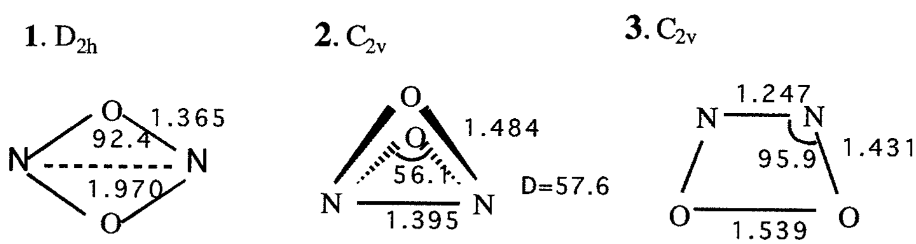
***Computer Resource:*** IBM SP2 [MHPCC DC]

***Research Objective:*** To support and guide experimental efforts to synthesize the high-energy isomers of NO dimer, $(NO)_2$. While there is indirect evidence for the existence of these molecules, they are metastable at best, so accurate theoretical studies are essential. Using the SP2 at Maui, we have mapped out extensive sections of the singlet and triplet potential energy surfaces for both isomers to aid in these synthesis efforts.

***Methodology:*** The potential energy surfaces for these isomers have been studied using multiconfigurational self-consistent field (MCSCF) wavefunctions, augmented by second-order perturbation theory, with large basis sets. These MCSCF calculations have a very large active space and are highly demanding computations that would have been impossible without access to the IBM SP2 at the Maui Center and without the development of the parallel version of GAMESS.

***Results:*** Of the four high-energy isomers first identified, one may be discounted due to rapid predissociation to $N_2O$ + O. The other three (see figure) appear to be stable in this regard. At this level of theory, isomers **1**, **2**, **3** are higher in energy than 2 NO by 49, 82, and 53 kcal/mol, respectively. The transition state for decomposition of 1 to 2 NO has been determined to lie 39 kcal/mol above 1. We find that the repulsive $^3A\leq$ state does indeed cross the ground singlet state before the transition state (that is, on the reactant side), but this crossing is predicted to occur at an energy that is about 32 kcal/mol above the reactant well. So, it is likely that isomer **1** exists and might be isolated. Although isomer **3** is planar, the transition state that leads to decomposition to 2 NO is twisted by about 15 degrees. The height of the dissociation barrier is estimated at about 20 kcal/mol. The lowest triplet state is 4 kcal/mol lower than the corresponding singlet. Although the triplet state is close to the singlet in energy in the transition state region, the triplet energy is much higher in the reactant channel. It is unlikely that in this case or in the case of the $D_{2h}$ isomer, the singlet-triplet crossing will prevent detection of isomer **3**. The primary result is the prediction that both isomers **1** and **3** should be possible to synthesize.

***Significance:*** This work is being done in connection with the Air Force High-Energy Density Materials program, which seeks to identify, characterize, and exploit high-energy density systems for use as advanced rocket propellants. The addition of high-energy molecules (such as the high-energy isomers of $N_2O_2$) to rocket fuels is expected to enhance significantly propellant performance, therefore leading to significant savings in launch costs.




*High-energy $N_2O_2$ isomers*

# Modeling Organic Matter Adsorbed onto Clay

J.D. Kubicki and S.E. Apitz
*Naval Command, Control and Ocean Surveillance Center, San Diego, CA*
*Office of Naval Research, Arlington, VA*

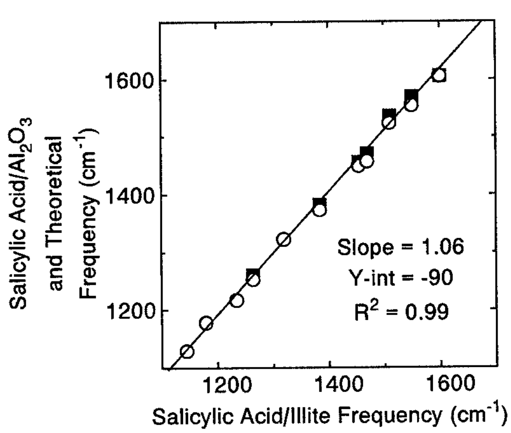
***Computer Resource:*** Cray 916 [CEWES MSRC]

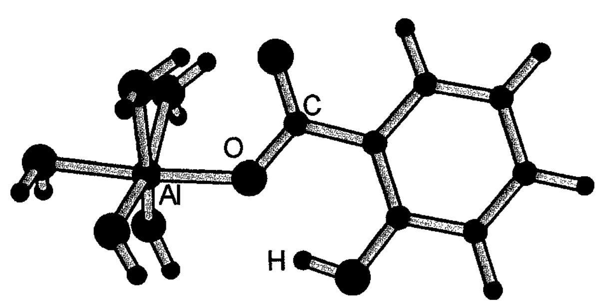
***Research Objective:*** To determine if chemical adsorption of organic contaminants onto minerals will decrease their potential environmental risk. Our research has focused on adsorption mechanisms of natural organic matter (NOM) onto minerals that make up a large percentage of sediments. Basic research is necessary in this area because NOM in sediments controls the transport and fate of nonpolar organic contaminants (NPOC), such as polycyclic aromatic hydrocarbons. The different forms NOM takes in nature have significant consequences for the transport and fate of NPOC. However, there has not been a great deal of research on the chemistry of NOM-mineral interaction at the molecular level.

***Methodology:*** We have conducted adsorption experiments with simple model compounds that contain organic functional groups similar to those present in NOM. This methodology allows us to interpret infrared spectra more readily than would be the case for complex mixtures of NOM. Infrared spectra of the adsorbed simple compounds can be modeled with molecular orbital calculations. We plan to use these assignments made on simple model systems to help interpret the spectra of more complex mixtures of NOM.

***Results:*** The combination of attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy and molecular orbital theory (figure on left) has allowed us to confirm the ester-like bonding mechanism proposed for salicylate onto alumina and clays (figure on right). Others had suggested that formation of C-O-Al bonds may be responsible for strong adsorption of NOM; the strong correlation (left figure) between experimental and theoretical frequencies generated from this molecular configuration (right figure) supports earlier conclusions based on bulk adsorption experiments of humic acid onto $Al_2O_3$ and clays.

***Significance:*** Determination of NOM bonding mechanisms onto clays is a first step toward understanding the molecular-level chemistry of organic contaminants in the environment. In this case, we have shown that stable complexes can form between NOM and mineral surfaces. Thus, organic contaminants intertwined with the NOM can be sequestered onto the mineral surface and lower the potential environmental risk below that predicted based on the total concentration of the contaminant alone. Spectra and modeling of contaminant-NOM interactions will further elucidate the chemical nature of the sequestration that occurs as contaminated sediments are aged.




*Comparison of salicylic acid/$Al_2O_3$ measured (red squares, figure on left) and theoretical (green circles; frequencies generated from the model structure on the right) to measured salicylic acid/illite (x-axis) frequencies demonstrates excellent correlations. Molecular model of salicylate bonded to $Al^{3+}$ on the right gives the best fit to observed vibrational frequencies as compared with numerous other possible sorption complexes*

# Explosive Capability of Chemical Agents CK and AC

B.M. Rice, S.V. Pai, and C.F. Chabalowski
*Army Research Laboratory, Aberdeen Proving Ground, MD*

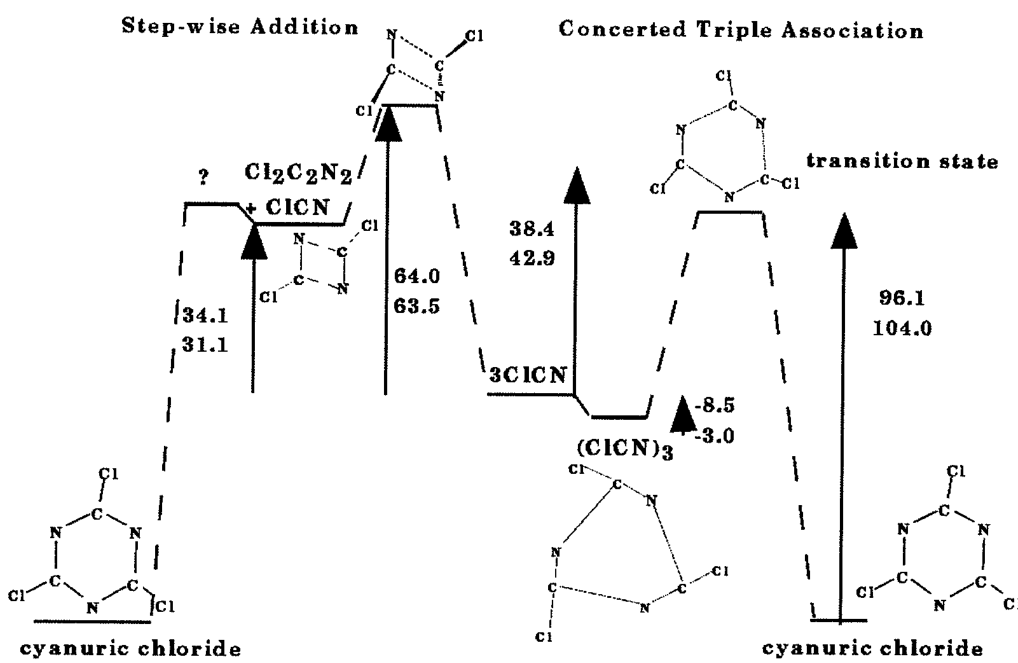
***Computer Resource:*** SGI Power Challenge Array [ARL MSRC]

***Research Objective:*** To characterize the polymerization reactions of chemical agents CK (ClCN) and AC (HCN).

***Methodology:*** Quantum mechanical methods were used to locate and characterize critical points on the potential energy surfaces for CK and AC. The large number of electrons and high level of theory used in these calculations required multiprocessing capabilities as well as the superior CPU and disk resources available on the SGI Power Challenge Array (ARL MSRC).

***Results:*** The low energy pathway for trimerization of CK and AC is an unusual concerted triple association reaction rather than a stepwise addition. The activation barriers for both systems are approximately 40 kcal/mol. Between 80 and 100 kcal/mol is released to the surroundings upon trimerization. A weakly bound trimer cluster acts as a pre-reaction intermediate that is structurally favorable to the concerted triple association, and removes the steric hindrance to the reaction. The large energy release is sufficient to initiate additional reactions and could explain explosions of containers of old CK and AC.

***Significance:*** Agents CK (ClCN) and AC (HCN) were standard and substitute fill, respectively, of chemical munitions during World War II. Excavation of abandoned chemical warfare munitions dumps for environmental cleanup has uncovered old munitions, some of which are assumed to contain CK or AC. As a result of the massive production of these munitions in the 1940s, it is expected that more CK and AC munitions will be uncovered in old disposal sites. These cyanide compounds are extremely toxic and must be destroyed. However, there are reports of explosions of old cylinders containing CK and AC. Our accomplishments in characterizing the polymerization reactions for CK and AC have confirmed that these reactions are extremely exothermic and thus have provided the information needed to direct safe handling of these old munitions.




*Zero-point corrected relative energies (kcal/mol) of critical points on the CK potential energy surface; similar features exist for the AC potential energy surface*

# Inner Life of Rust

G.A. Voth
*University of Pennsylvania, Philadelphia, PA*
*Office of Naval Research, Arlington, VA*

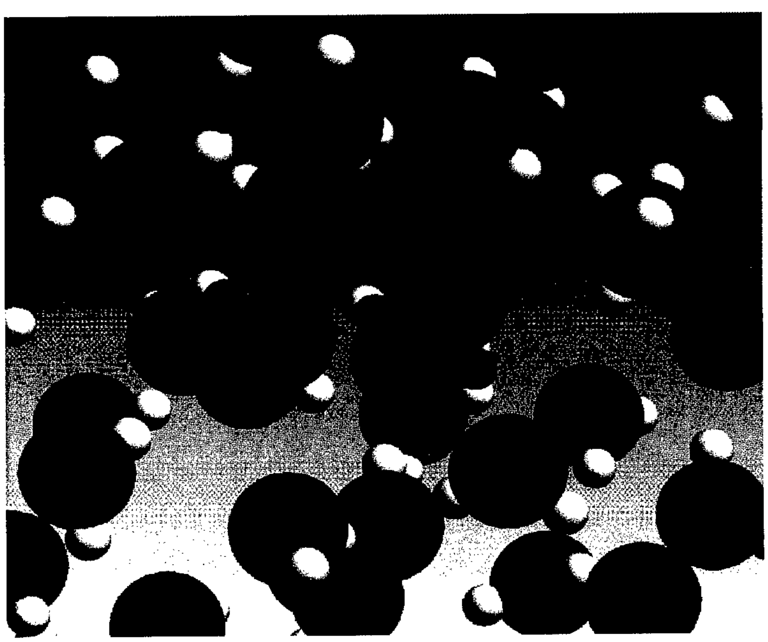
***Computer Resource:*** Cray C90 [Pittsburgh Supercomputing Center], IBM RS/6000 [MHPCC DC], and SGI Power Challenge [University of Pennsylvania]

***Research Objective:*** To investigate the rate, energetics, and dynamics of electron transfer across an electrode/electrolyte interface. This is a fundamental step in the corrosion process and also in the reactions involved in electrical storage batteries.

***Methodology:*** An iron ion in water at 300 degrees Kelvin has been simulated interacting with the surface of a platinum electrode. To represent realistically the ion's interactions with the water around it, the simulation included 671 water molecules. The first part of the work applied an essentially Newtonian scheme for calculating the forces between atoms. The next phase treated the water quantum mechanically, which meant quantizing the hydrogen nuclei of each water molecule. The Feynman path integral technique was used, an approach to quantum computations that was adapted to predict the rate of electron transfer processes. This formalism allows the inclusion of the diffuse nature of a quantum hydrogen and the zero-point energy of the O-H bonds within a molecular dynamics simulation.

***Results:*** The free energy of electron transfer as a function of three different reaction coordinates was calculated. The reaction coordinate was shifted in each of several choices, but the features of the free energy curve remained approximately the same. The path integral molecular dynamics calculation showed that the free energy and rate of electron transfer is very different for the quantum water model. The driving force for the oxidation reaction is much higher for the quantum water model. This illustrates the importance of the quantum effects from the solvent in the electron transfer process.

***Significance:*** A microscopic understanding of this process will aid development of more efficient batteries and rust-resistant processes that can reduce the estimated $10 billion annually spent in the United States on rust prevention and repair.



*Snapshot from a CMD simulation of the proton transfer complex (blue and green) in water (red and white)*

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### Modeling Organic Matter Adsorbed onto Clay

J.D. Kubicki, M.J. Itoh, and S.E. Apitz, "Ab Initio Model of Salicylate Adsorbed Onto $Al_2O_3$ and Illite Clay," *Abstracts of the American Chemical Society* **210** (1996).

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### Explosive Capability of Chemical Agents CK and AC

S.V. Pai, C.F. Chabalowski, and B.M. Rice, "Ab Initio Study of Reactions of *sym*-Triazine," *Journal of Physical Chemistry* **100**(14) (1996).

# Computational Electromagnetics and Acoustics

*Computational Electromagnetics and Acoustics (CEA) uses high-resolution algorithms to simulate diffraction, refraction, and interaction phenomena in electromagnetic and acoustic fields. Modeling for antenna array, signature prediction, and the performance of microwave devices requires the development of scalable numerical procedures for governing equations with well-posed initial and boundary conditions and a discretized geometric definition of the scatterer.*

*The accomplishments in CEA presented here represent three distinct categories including novel DoD mission applications, state-of-the-art applications of concurrent computing, and innovative numerical algorithms that will be used to further increase simulation capability. In particular, the high-fidelity radar-cross-section and navigation antenna computations for fixed-wing aircraft have pushed the simulation envelope to include previously unattainable frequency spectra and configuration complexity. The overall technical achievements also reflect a wide spectrum of defense applications in signature processing, navigation antennas, high-power microwave devices, and sonar systems.*

Dr. Joseph J. S. Shang
Wright Laboratory
Wright-Patterson AFB, OH
CTA Leader for CEA

# Combat Aircraft Simulation

D.D. Car and J.M. Putnam
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*Air Force Office of Scientific Research, Washington, DC*

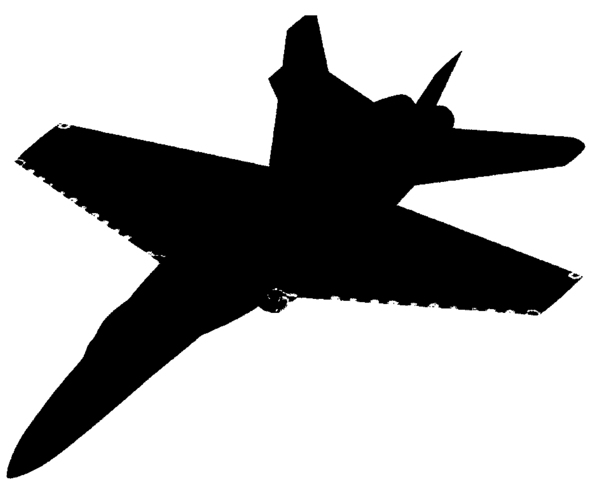
***Computer Resource:*** Intel Paragons XP/S MP 45 [MDA] and Intel Paragon [ASC MSRC]

***Research Objective:*** To demonstrate the scalability on a massively parallel computer of the method of moment (MoM) based CARLOS derivative codes in a full-scale simulation of the radar cross sections (RCS) and navigation antennas on the F/A-18 C and F-15 aircraft, respectively.

***Methodology:*** In these simulations, the electromagnetic interactions were formulated in terms of discretized integro-differential equations solved by the MoM (Galerkin) procedure. For the RCS simulation of the F/A-18, the aircraft was modeled with 74,818 facets, which translates to 228,480 unknowns; the F-15 antenna calculation required fewer unknowns. For computational efficiency, in the RCS simulations, physical symmetry was used to reduce the problem to two dense matrix systems of rank 114,240.

***Results:*** These problems were solved on the Paragon supercomputer with 196 multiprocessing (MP) compute nodes having 64 Mbytes of memory on each node. The Intel ProSolver-DES dense equation solver routines were used. Large, dense matrices typically require swapping out the matrix to disk. In this case, the supercomputer was configured with 10 SCSI-16 RAID units to yield a disk space of 168 Gbytes. For the RCS calculations, two polarizations for 181 illumination angles were computed. Representative results of these simulations are shown in the accompanying figures depicted as current images.

***Significance:*** The efficacy of the CARLOS family of codes on a massively parallel supercomputer has been demonstrated for the simulation and design support of complex weapon platforms. McDonnell Douglas Aerospace's experience shows that the Paragon implementation of the CARLOS derivative codes can provide a 5- to 10-fold design cycle time compression. Under sponsorship of the national Electromagnetic Code Consortium, the CARLOS-3D RCS code is presently in use at approximately 100 NASA, DoD, and contractor sites.



*Current image of F/A-18C for nose-on illumination (500 MHz)*

*Current image of F-15 tail-mounted navigation antenna*

# Jet Engine Scattering and Conformal Antenna Radiation

J.L. Volakis, A. Chatterjee, D.C. Ross, M.D. Casciato, and J. Gong
*University of Michigan, Ann Arbor, MI*
*Naval Air Warfare Center, China Lake, CA*

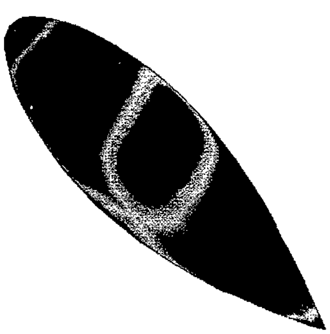
***Computer Resource:*** Intel Paragon [ASC MSRC]

***Research Objective:*** To develop numerical methods and associated design-oriented computer codes to analyze electromagnetic scattering (radar cross section) by airborne substructures and to evaluate the performance of antennas and onboard communication systems.

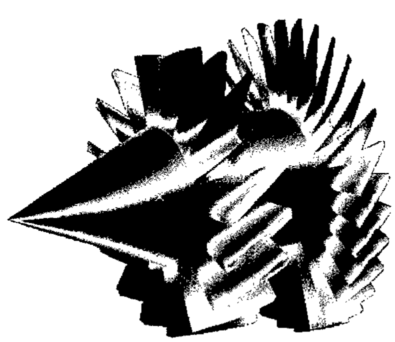
***Methodology:*** The finite-element method (FEM) is used to simulate the electromagnetic phenomenology associated with radar scattering from aircraft, including engines, and for robust characterizations of antenna and microwave circuit parameters. In contrast to integral equation approaches, the FEM allows the simulation of a large class of structures and devices without limitations caused by geometrical adaptability and material composition.

***Results:*** The three-dimensional scattering code FEMATS was improved with the incorporation of new conformal absorbing boundary conditions, which has led to substantial reduction in degrees-of-freedom and processor requirements. This permitted the modeling of practical configurations using more than 0.5 million unknowns and run times of 20 minutes or less at 300 Mflops. FEMATS was parallelized on the Intel Paragon and IBM SP-2 with nearly linear scalability; matrix compression techniques proved very successful for vectorization on the C916. The NASA almond fields were calculated using FEMATS. A most important development was the completion of a new jet engine analysis code FEMENG. Developed to run on the Paragon, this is the first code capable of such analysis. It required the development of innovative domain decomposition approaches to overcome difficulties resulting from engine complexity and size. Exploitation of the engine blade periodicity, identification of dominant mode fields, and new mesh truncations using artificial absorbers all played a crucial role in the development of a code capable of practical simulations. These codes were used to study the effect of new materials and geometries aimed at size reductions, increased bandwidth, and gain. A third finite-element code FEMA-PRISM was improved for conformal antenna analysis and design (right-hand figure).

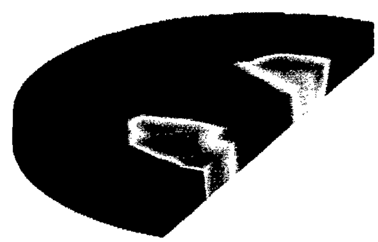
***Significance:*** This project represents the development of leading-edge design and analysis electromagnetics software for radar scattering by composite aircraft and for antenna design. Requirements for new antenna designs are rapidly increasing as a result of the proliferation of personal communication systems. This software is important for both military and commercial applications.



*Magnetic field strength on the surface of the 1-m NASA almond (metallic body of the shown shape) for the vertical polarization. Note oscillation due to creeping wave phenomena.*



*Magnetic field distribution on the first two stages of a jet engine due to single mode excitation*



*Field strength around a dual-patch antenna excited at resonance*

# High-Resolution Modeling of a Magnetically Insulated Line Oscillator

1st Lt. J.J. Havranek, Capt. B.J. Smith, and 2nd Lt. M.A. Anderson, U.S. Air Force
*Phillips Laboratory, Kirtland AFB, NM*

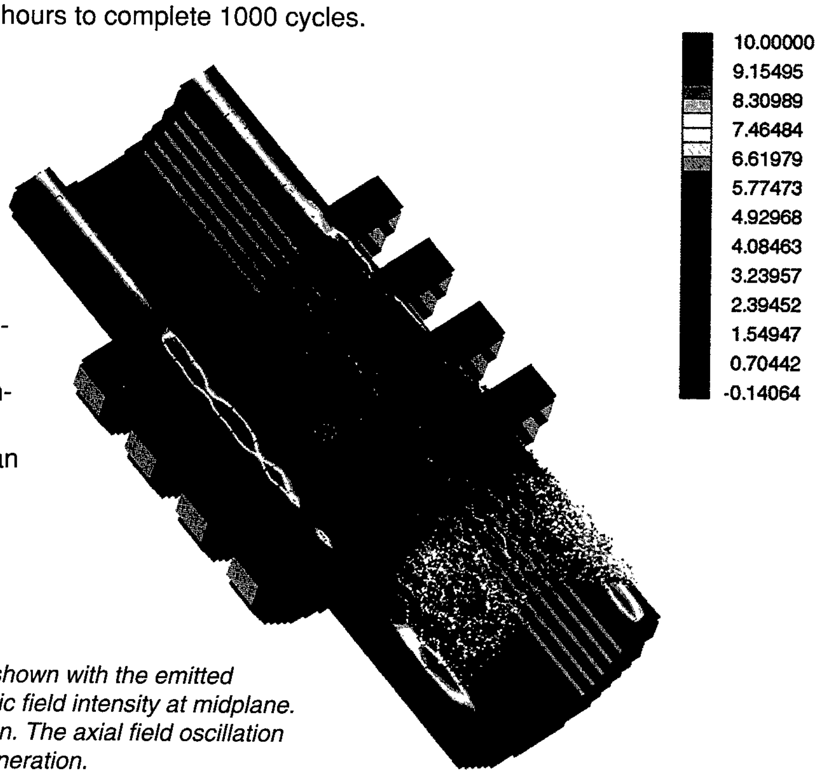
***Computer Resource:*** IBM SP2 [MHPCC DC]

***Research Objective:*** Because of memory and time constraints on serial computers, researchers interested in microwave devices have been unable to simulate physical domains either as large or as finely resolved as they would like. We have developed a three-dimensional parallel particle-in-cell code that puts much more computational power into the hands of computational scientists, freeing them from these constraints.

***Methodology:*** We solve Maxwell's equations on a staggered mesh using the standard, explicit, finite difference time domain (FDTD) algorithm. The plasma is represented by many "super-particles," which move within the FDTD mesh. The fields interact with the particles through the Lorentz force, and the particles affect the fields by weighting the particles' currents onto discrete location on the mesh. For use on parallel platforms, both 1-D and 3-D partitioning have been implemented. The ability to dynamically rebalance the problem has been added and is found to decrease run times. For parallel communication, we have written our own message-passing library, which includes parallel I/O capabilities. This library is written on top of both Parallel Virtual Machine (PVM) and Message Passing Interface (MPI). The flexibility of choosing different low-level message-passing libraries coupled with standard ANSI C programming makes the code extremely portable.

***Results:*** One of the earliest uses of our parallel code was the simulation of a magnetically insulated line oscillator (MILO). A 4 MV potential is applied across a coaxial gap, causing field emission of electrons from the inner conductor. The magnetic field created by the electrons' own current prevents the beam from shorting across the coaxial gap. The figure shows a cutaway of the MILO geometry with the electric field intensity indicated at the midplane and a scatter plot of the particles above. The data shown belong to a reduced data set of a 200,000 cell problem with 400,000 particles. The simulation ran on 8 nodes of the IBM SP2 and took less than 1.5 hours to complete 1000 cycles.

***Significance:*** The investigation of high-power microwave devices is a high priority for the U.S. weapons program, and there are many outstanding issues to be studied. Phenomena such as mode competition and power loss at interfaces have yet to be addressed adequately. High-resolution 3-D simulations are needed to help understand these and other impediments to high-power microwave production before this important weapon technology can be developed fully.




*The lower half of the MILO geometry is shown with the emitted electrons in the upper half and the electric field intensity at midplane. The data are from 5 ns into the simulation. The axial field oscillation indicates the beginning of microwave generation.*

# Plasma Asymmetry in a 3-D World

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*Phillips Laboratory, Kirtland AFB, NM*
*Air Force Office of Scientific Research, Washington, DC*

***Computer Resource:*** IBM SP2 [MHPCC DC]

***Research Objective:*** The real-world case of three-dimensional simulation of a magnetofluid has, until now, been out of reach of researchers in plasma physics because the complexity of serial 3-D computation overwhelms both serial computer hardware and the patience of scientists. Parallel Mach3 adds time-dependent 3-D collisional plasma simulation to the scientist's toolbox.

***Methodology:*** Parallel Mach3 solves the unsteady, single-fluid, resistive magnetohydrodynamic (MHD) equations on a 3-D mesh composed of arbitrarily shaped hexahedral cells in an operator split manner. All but the convective operators are solved implicitly so the Courant condition can be exceeded without exciting numerical instabilities. Finite volume differencing permits the computational mesh to be nonorthogonal. Mach3's multiple block structure allows for simulation of complex geometric configurations, and parallelization is accomplished by distributing $n$ blocks among $p \leq n$ processors. Interblock communication is accomplished via the Message Passing Interface (MPI), which ensures that Parallel Mach3 is portable to most high performance computer platforms.

***Results:*** To illustrate the power of Parallel Mach3, we have performed the first 3-D simulated implosion of a solid-core gas puff. This krypton $z$-pinch is driven by a high-energy electric discharge from a 5 MV Marx Bank. The initial density is seeded with an $m = 4$ azimuthal and a $k = 2$ axial perturbing mode. The figure below shows the mass density 50 ns into the implosion when it has been heated to the plasma state and is well into the nonlinear regime of instability growth. This simulation used 140,000 computational cells, which is too large to fit on most single-node machines, and took 10 hours on 20 nodes of the IBM SP2 with a parallel efficiency of about 75%.

***Significance:*** The Rayleigh-Taylor instability is a problem that limits the performance of a wide range of plasma systems of interest to DoD including explosively driven pulsed systems, space plasmas, and radiation sources. Three-dimensional simulations of fast $z$-pinch implosions are allowing researchers to understand the nonlinear phase of instability growth. This represents a major contribution to the field of plasma physics, which will lead to enhanced performance of advanced DoD systems.


*Cut planes and isosurfaces of mass density (in kg/m³) of radially compressing plasma at 50 ns. The classical Rayleigh-Taylor spike and bubble pattern is easily recognized. The strong azimuthal variations are an indication of important 3-D physics.*

# Femtosecond Nonlinear Optical Probes of Microscopic Many-Body Interactions

J.V. Moloney and R.A. Indik
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*Air Force Office of Scientific Research, Washington, DC*

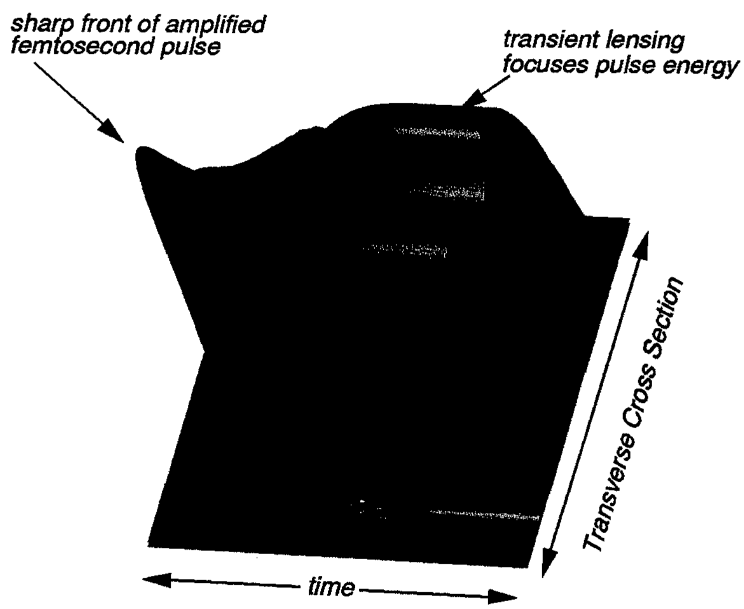
***Computer Resource:*** IBM SP2 [MHPCC DC]

***Research Objective:*** To build a physically and mathematically self-consistent, robust hierarchy of models of high-power semiconductor amplifiers and lasers, based on the microscopic many-body physics of the interaction of light with semiconductor media. A goal of the project was to be able to a priori design and optimize complex laser structures before resorting to expensive device fabrication.

***Methodology:*** The Maxwell-Semiconductor Optical Bloch equations provide a quantitative description, on a microscopic level, of the complex many-body interactions of carriers (electrons and holes) in two or more component plasmas. Ultrafast physical phenomena, such as bandgap renormalization, Coulomb interactions, heating, and memory effects, all significantly affect the macroscopic response of the material to an incident light field. The problem, ideally suited to the coarse-grained parallelism of the IBM SP-2 architecture at MHPCC, utilizes a domain decomposition enabling individual nodes (64 nodes are typically used) to carry out intensive computation on the many-body Bloch equations while nearest neighbor coupling (diffraction) in the Maxwell part involves minimal communications overhead.

***Results:*** The figure shows a single snapshot of the intensity (violet) and (negative of) the carrier density (green) distribution at a fixed location along a broad area semiconductor amplifier. The initially heated plasma cools, causing amplification on the trailing edge of the pulse, leading to strong distortion, while a transient self-focusing induced lens focuses the center of the pulse.

***Significance:*** Semiconductor lasers and high-power amplifiers provide compact integrated structures for a wide range of industrial and military applications. For example, new pulsed laser sources offer many military opportunities such as space-based high bandwidth satellite communications, laser rangefinders, active laser countermeasures, and remote sensing.




*Snapshot of transient lensing*

# High-Frequency Acoustic Time Series Simulation

X. Zabalgogeazcoa and P. Lallement
*Alliant Techsystems, Arlington, VA*
*Oceanographer of the Navy, Washington, DC*

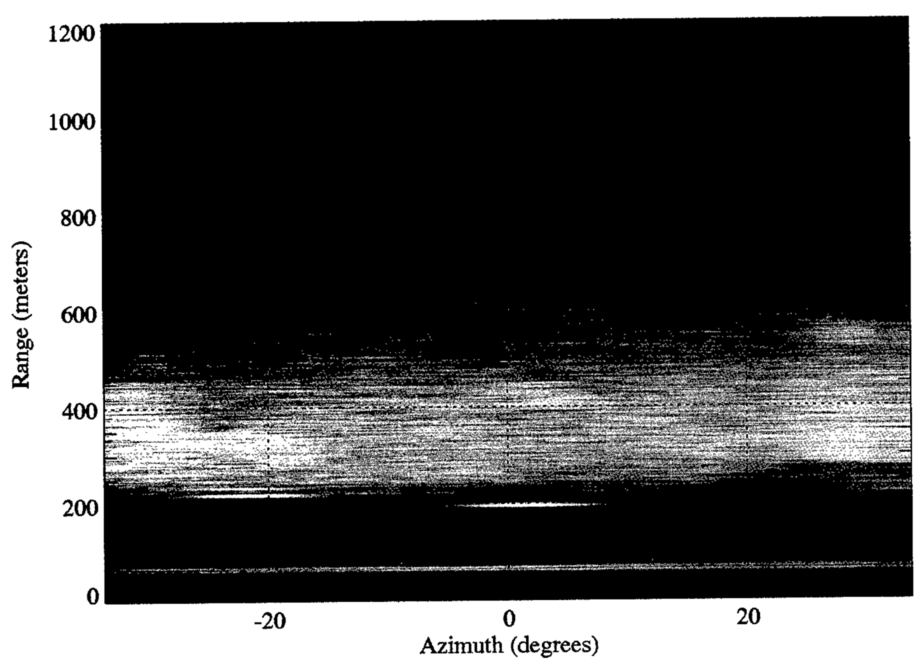
***Computer Resource:*** Intel Paragon [NCCOSC DC]

***Research Objective:*** To create a high-fidelity, computer-generated representation of a high-frequency, range-dependent acoustic environment designed to allow the immersion of actual sonar systems in realistic scenarios and acoustic propagation conditions.

***Methodology:*** The key to the utility of the High-Frequency Acoustic Time Series Simulator (HF-ATSS) lies in the detailed realism of the environmental components of the simulated signals. Full-spectrum realizations of source waveforms are propagated coherently through environments in which bathymetry, bottom type, and sound speed are range and azimuth dependent. For active sonar scenarios, bottom reverberation is created for either mono- or bistatic configurations. The HF-ATSS architecture allows the real-time synthesis of sensor or beam-time series for unscripted scenarios so that actual sensor processors can be integrated into a simulated context. Operators can then interact with their actual displays in a realistic dynamic operating environment. Alternatively, pre-scripted scenarios may be used for test and evaluation of prototype signal and information processing systems in controlled and repeatable high-fidelity synthetic environments. Navy standard databases and physics-based propagation models are used for realistic representation of the underwater environment.

***Results:*** HF-ATSS is used to create acoustic data for stimulating the AN/SQQ-32(v) Minehunting Detection Sonar. The synthetic data have been compared qualitatively and statistically to a limited set of actual SQQ-32 data collected during the sonar's operational evaluation. The synthetic data reflected the proper sensitivity to the given acoustic environment and exhibited similar characteristics in terms of signal content. HF-ATSS is installed on the NCCOSC Paragon, where it is used to create time series to drive the SQQ-32 B-scan displays in a real-time, interactive, free-play scenario.

***Significance:*** HF-ATSS provides the acquisition and development communities with a high-fidelity simulation tool to be used in applications such as realistic operator proficiency training, shallow water active signal processing algorithm development, and simulation-based sonar design.




*SQQ-32 data created by HF-ATSS, showing bottom reverberation and two targets*

# Modeling of Multistage Frequency Conversion in Optical Parametric Oscillators

G.T. Moore and K. Koch
*Phillips Laboratory, Kirtland AFB, NM*

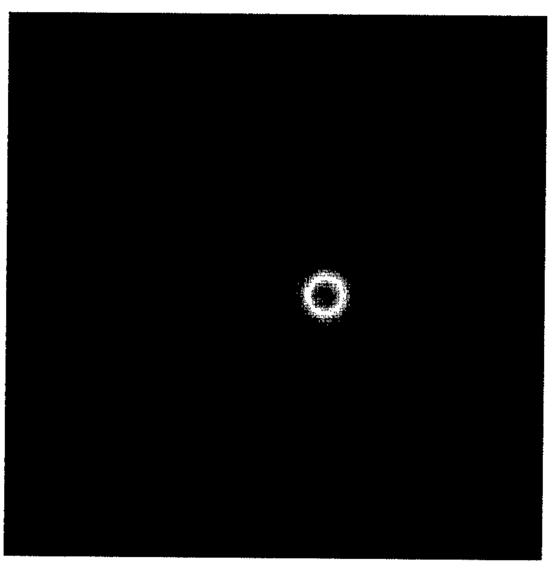
***Computer Resource:*** Cray Y-MP [CEWES MSRC]

***Research Objective:*** Multistage intracavity frequency conversion in optical parametric oscillators (OPO) is a promising method for efficiently and tunably generating new optical wavelengths, starting from a pump laser of fixed wavelength. Plane-wave analyses, which consider only the longitudinal dimension, give useful, but limited, information on promising dynamical regimes. Numerical modeling, which includes one or more of the transverse spatial or temporal dimensions, provides a detailed picture describing effects such as walk-off, diffraction, cavity focusing, beam quality, group-velocity mismatch, group-velocity dispersion, cavity-length desynchronization, and cavity or pump misalignment.

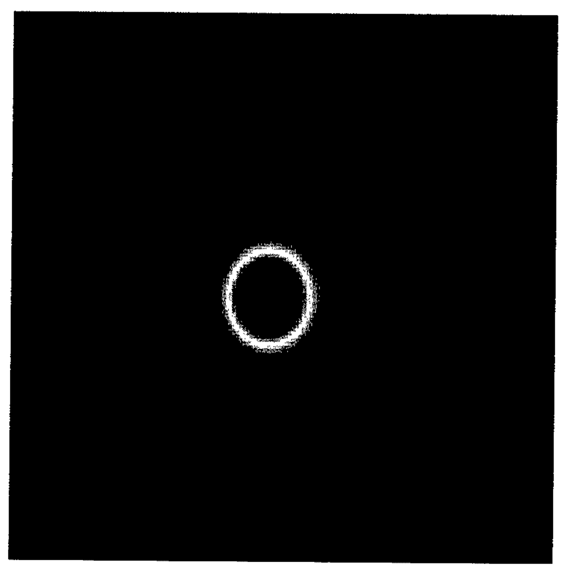
***Methodology:*** Multipass codes have been developed that solve the three-wave- or two-wave-mixing equations using fast Fourier transform (FFT) beam propagation and fourth-order Runge-Kutta integration. One code treats a single transverse or temporal dimension; the other code treats both spatial dimensions. Full four-dimensional modeling has not been attempted, but might be practical with parallel processing.

***Results:*** A number of multicrystal devices have been modeled, and it has been found that often the high-efficiency conversion predicted by plane-wave theory also occurs in higher dimensional simulations. Cases where effects such as walk-off or cavity focusing decrease the efficiency or produce unstable operation can also occur. As an example, the figure below shows steady-state intensity profiles for a device designed to produce sodium resonance radiation by intracavity sum-frequency generation of the 1.064 μm pump and 1.319 μm signal of a silver gallium sulfide OPO. The power conversion efficiency to 589 nm is 79%. A similar experimental device was operated at 15% efficiency at lower peak pump power. Numerical simulations converge rapidly at high pump power, but require many passes when close to threshold. The figure shows the near field of the depleted pump and the far field of the 589 nm light.

***Significance:*** Multistage frequency conversion in OPOs pumped by Nd:YAG lasers provides an efficient all-solid-state technology for generating desired infrared or optical wavelengths. For example, a bright source of sodium resonance radiation is needed for generating an artificial guide star for adaptive-optics imaging.



*Pump near-field width = 625 μm*



*Yellow far field of view = 7.54 mrad*

# Parallel Computing in Computational Electromagnetics

V. Shankar, W.F. Hall, C.M. Rowell, and A. Mohammadian
*Rockwell International Science Center, Thousand Oaks, CA*
*Army Research Laboratory, Aberdeen Proving Ground, MD*
*Air Force Office of Scientific Research, Washington, DC*

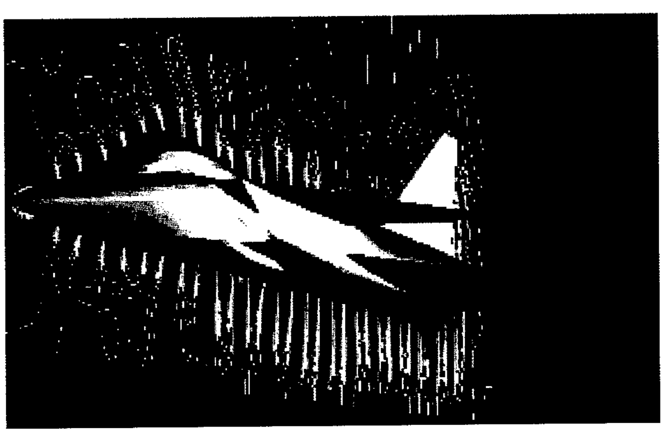
***Computer Resource:*** Intel Paragon [ASC MSRC], Cray C916 [CEWES MSRC], and IBM SP2 [MHPCC DC]

***Research Objective:*** To develop a massively parallel version of a time-domain computational electromagnetics (CEM) solver to compute the radar cross section (RCS) of electrically large targets (typical fighters at 100 MHz to 20 GHz) and demonstrate the scalable and transportable performance on a number of parallel machines, such as Intel, Cray T3D, SP2, and nCUBE.

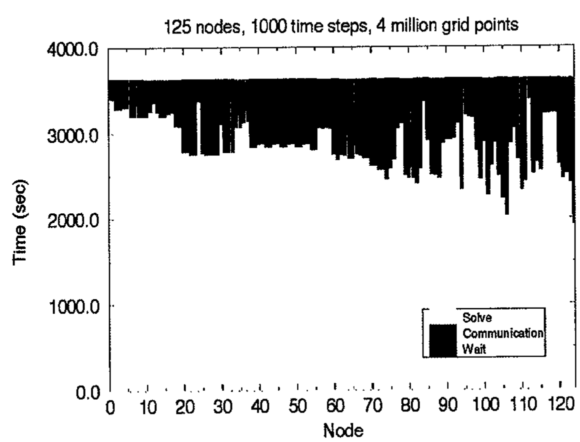
***Methodology:*** A finite-volume, time-domain Maxwell solver, originally developed for Cray-like vector machines, has been ported to massively parallel architectures using Message Passing Interface (MPI) libraries. The solver and the domain decomposition procedures accommodate both structured and unstructured grid arrangements. The solver is based on an explicit time discretization scheme that parallelizes very well, requiring less than 3% overhead for message passing.

***Results:*** The code RCSMPP runs on a number of platforms such as the Intel Paragon, Cray T3D, nCUBE, and the IBM SP2. Use of the MPI libraries allows execution of the code not only on massively parallel machines but also on workstation clusters. The code has been demonstrated for computing the RCS of a complete fighter at 1 GHz requiring over 5 million grid points and 128 nodes of a Paragon. If one uses all the available nodes and memory on the IBM SP2, a problem size approaching nearly 200 million grid points can be computed.

***Significance:*** CEM is a critical technology in the advancement of future aerospace development through supercomputing. As we transition from the present Gflops to the next generation Tflops computing, CEM will become integral to aerospace design not only as a stand-alone technology but also as part of the multidisciplinary coupling that leads to well-optimized designs.



*Parallel computation of scattered fields from a fighter for RCS prediction*




*Parallel performance of RCSMPP on a 128-node Paragon*

# Solutions of Hyperbolic Systems of Partial Differential Equations on Distributed Memory Parallel Computing Platforms

Capt. D.C. Blake and Maj. T.A. Buter, U.S. Air Force
*Air Force Institute of Technology, Dayton, OH*
*Wright Laboratory, Wright Patterson Air Force Base, OH*

***Computer Resource:*** Intel Paragon [ASC MSRC], IBM SP2 [MHPCC DC], and Cray T3D [AFDTC DC]

***Research Objective:*** To develop algorithms and techniques for numerically solving the Maxwell and Navier-Stokes equation sets in distributed memory parallel computing environments with a focus on the design of aerospace systems having desirable aerodynamic and electromagnetic signature properties.

***Methodology:*** An application framework has been developed that abstracts many aspects of parallel algorithm development and accepts a wide range of partial differential equation solvers. This application framework, in conjunction with a finite-volume time-domain (FVTD) Maxwell equations solver, was then used for an in-depth examination of domain decomposition approaches for mapping grid-based computational fluid dynamics and computational electromagnetics problems to massively parallel machines.

***Results:*** Accurate numerical simulations of the electromagnetic fields surrounding oscillating electric dipoles and inside rectangular waveguides have been performed. In addition, the scattering behavior and associated radar cross section have been examined for perfectly electrically conducting spheres. Techniques have been developed that facilitate rapid porting of parallel programs between various distributed architectures and message passing libraries, including Intel's NX as well as Message Passing Interface (MPI) and Parallel Virtual Machine (PVM). The performance of various domain decomposition techniques on several modern distributed memory parallel computing platforms has been quantified thus allowing for much more efficient use of such machines.

***Significance:*** Accurate simulation of complex aerodynamic and electromagnetic phenomena is of fundamental importance in the design of future aerospace systems. Traditionally labor-intensive simulation and design can be effectively accomplished through the use of massively parallel computing platforms in conjunction with efficient algorithms designed to solve the Maxwell and Navier-Stokes equations in an integrated manner.

*Magnitude of scattered electric field surrounding a perfectly electrically conducting sphere*

# AIM — Fast Electromagnetic Simulation Algorithm for Massively Parallel Computer Platforms

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*North American Aircraft, Rockwell International, Los Angeles, CA*
M.K. Bleszynski
*Rockwell International Science Center, Thousand Oaks, CA*
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

***Computer Resource:*** Intel Paragon [ASC MSRC] and IBM SP2 [MHPCC DC]

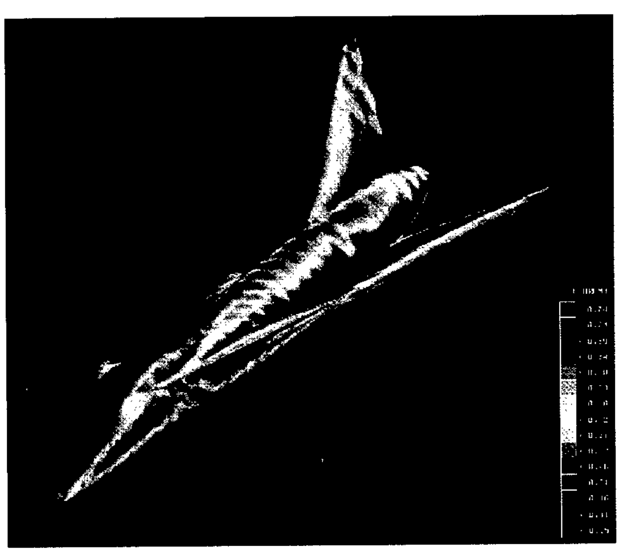
***Research Objective:*** To develop efficient and highly accurate computational tools to simulate and study electromagnetic problems of interest for defense and commercial applications. In particular, to develop a scalable, massively parallel electromagnetic scattering code ultimately capable of predicting the electromagnetic signature of a real-size fighter aircraft or a missile at radar frequencies within the timeframe of hours.

***Methodology:*** The Adaptive Integral Method (AIM) is a novel algorithm for the simulation of large-size electromagnetic problems. It retains the accuracy of the numerically exact conventional (e.g., method of moments) solution methods while significantly reducing the required memory and solution time. The memory and solution time reduction is achieved by employing a compression technique based on a decomposition of the integral kernel of Maxwell's equations into the near- and far-field components. The parallel version of the AIM solver was developed and optimized for the Intel Paragon and IBM SP2 supercomputers.

***Results:*** The radar signature computations for the VFY218 fighter aircraft, perfectly conducting and coated with radar absorbing materials, were performed at frequencies of 100 and 300 MHz on the Intel Paragon and IBM SP2 parallel supercomputer platforms. The following code performance was obtained on the Intel Paragon:

| Frequency | Number of Unknowns | Number of Processors | Solution time |
|---|---|---|---|
| 100 MHz | 9,000 | 30 | 2 hours/(180 incident angles) |
| 300 MHz | 70,000 | 100 | 20 hours/(360 incident angles) |

***Significance:*** Model building and testing of low observable airborne vehicles are prohibitively expensive and time consuming. When completed, this work will provide a computational simulation tool that will reduce the cost and the time span of a design cycle of an airborne vehicle. It will also increase the number of concepts that can be evaluated in search of the best performing and most cost effective design.



*With the AIM code, one can compute distribution of electromagnetic fields on the surface of an aircraft and identify "hot spots," which constitute dominant contributors to the radar signature. Shown here are "hot spots" on the VFY218 fighter illuminated by a radar beam of 300 MHz.*

# New Tools for Electromagnetics Simulations

J.S. Shang
*Wright Laboratory, Wright-Patterson Air Force Base, OH*

***Computer Resource:*** Intel Paragon [ASC MSRC], Cray C916 [CEWES MSRC], IBM SP2 [MHPCC DC], and Cray T3D [AFDTC DC]

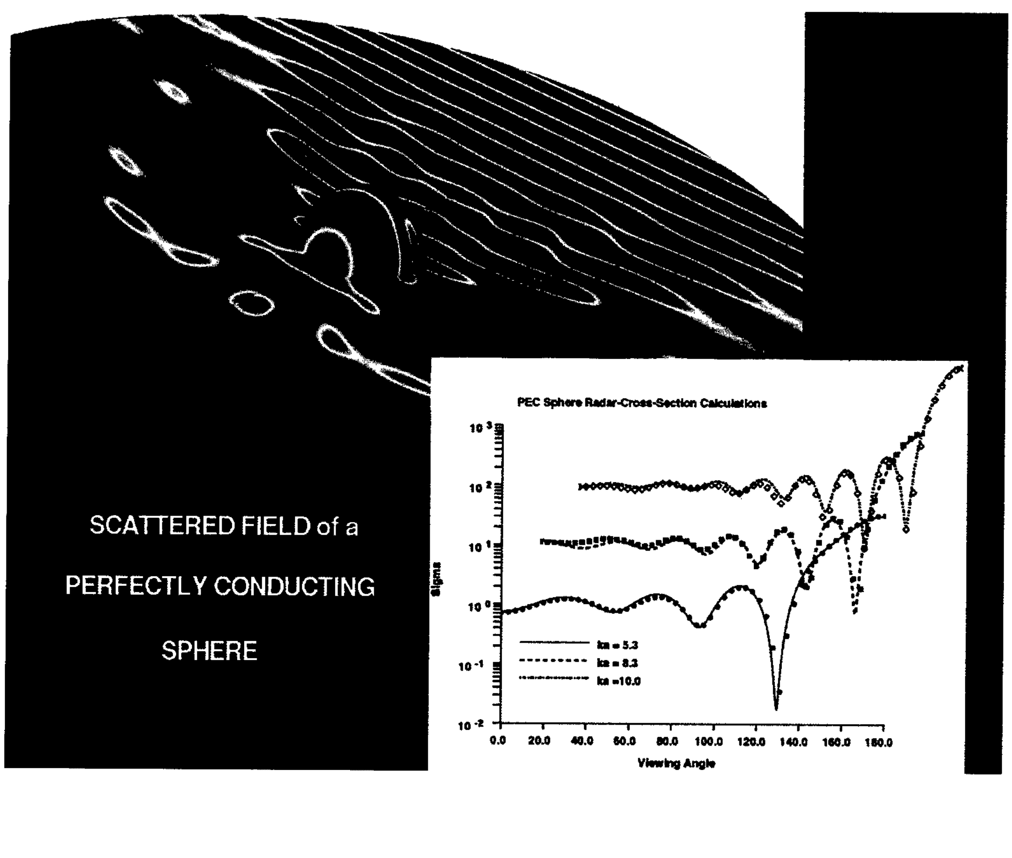
***Research Objective:*** To expand the simulation capability via first principles for electromagnetic signature, communication, and biomedical technology; to develop characteristic-based algorithms for solving the Maxwell equations in the time domain on massively parallel computers; and to validate numerical results for physical fidelity and engineering affordability.

***Methodology:*** The three-dimensional, time-dependent Maxwell equations are solved by using the characteristic-based formulation. The created numerical algorithms include a bidiagonal compact difference and a MUSCL type finite-volume scheme. Both schemes are temporally fourth-order and spatially third-order accurate windward biased approximations to mimic the wave propagation according to the zone of dependence. In porting the computational procedures for scalable performance, the load balancing was achieved by several domain decomposition approaches. The internodal communication is minimized through a range of varying data partitions for message passing operations.

***Results:*** The parallelized performance was verified by calculated radar cross sections (RCS) of a perfectly electric conducting sphere over a wide range frequency spectrum. The characteristic-based methods have proven to be numerically accurate and robust. The bistatic RCS of both horizontal and vertical polarization are predicted accurately to within a fraction of 1%. The scalable performance of the software has also been achieved over 240 computing nodes on three multicomputers.

***Significance:*** The characteristic-based numerical procedures have enlarged the numerical resolution wavenumber range significantly into higher frequency spectra. Meanwhile, the computing resource requirements for these RCS calculations have been reduced by a factor of 5.14 in comparison with results of one year ago. Now a group of wideband embedded antenna performance and missile RCS measurements can be verified on computers.

*Radar cross-section simulation*



# Computation of Scattered Electromagnetic Fields from Cylinders, Cavities, and Inlets


Y.S. Weber

*Wright Laboratory, Wright-Patterson Air Force Base, OH*

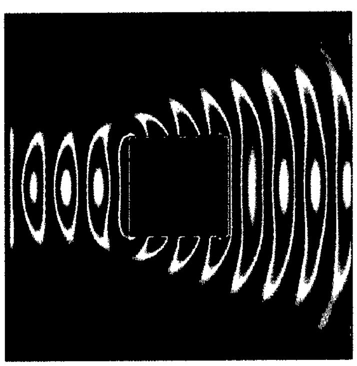

***Computer Resource:*** Cray C916 [CEWES MSRC]

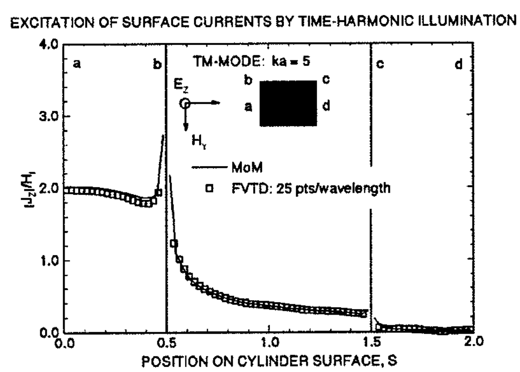
***Research Objective:*** To develop technology for accurately simulating electromagnetic scattering from air vehicles and their components by developing and applying high-order algorithms to solve the Maxwell equations. These algorithms reduce the resolution requirements dictated by standard second-order numerical integration techniques. This research is essential for the technology to become viable for computing the radar cross section (RCS) of full-scale configurations at realistic radar frequencies.

***Methodology:*** Characteristic-based finite-volume algorithms are transferred from the computational fluid dynamics community and applied to canonical configurations. Solutions to canonical configurations are generated and validated with benchmark data obtained from method of moment (MoM) computations. The results are analyzed with respect to dissipation, dispersion, and anisotropy. The influence of boundary conditions, domain size, and resolution on the quality of the solution is also investigated.

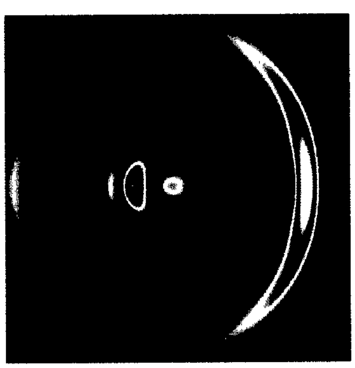
***Results:*** Several high-order, finite-volume, time-domain (FVTD) methods have been implemented for the numerical simulation of electromagnetic scattering from cylinders, cavities, and inlets. The surface currents and bistatic RCS have been validated with benchmark data from the MoM for infinite cylinders. For cavities, both monostatic and bistatic cross section as well as surface currents have been validated by comparisons with limiting physical optics treatments and data obtained from MoM. Wideband pulses have been used for incident TM- and TE-mode excitation to produce multiple-frequency responses. It has been found that backscatter cross section may be accurately obtained within 2% at 8 cells per wavelength using a fourth-order Runge-Kutta technique for the temporal integration coupled to a third-order MUSCL scheme for spatial integration.

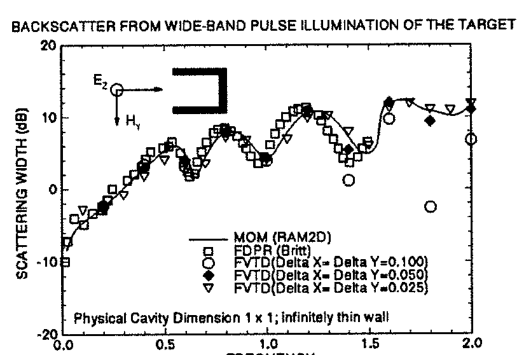
***Significance:*** Development of the simulation technology provides the ability to predict the radar signature of vehicles and subsystems. This technology can also be used for antenna design and biomedical applications.






*Computation of TM-mode electromagnetic scattering from cylinders and cavities using both time-harmonic and wideband inputs for illumination of the target*





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# Climate/Weather/ Ocean Modeling

*Research in the Climate, Weather, and Ocean (CWO) Modeling computational technology area is concerned with the accurate numerical simulation and forecast of the atmospheric and oceanic variability for both scientific and operational use. CWO is used on a daily basis within the DoD for safety of flight and safety at sea; mission planning and training (air, ground, sea, and space); optimal aircraft and ship routing; and weapon system design.*

*These CWO success stories were chosen to illustrate this diversity of application. For example, the lead success story of Hurlburt et al. demonstrates the critical role of model resolution in understanding the coupling between the ocean and topography. The Air Force Office of Scientific Research-sponsored success story of Professor Krisnamurti and the story of Van Tuyl and Rohaly both address the concept of physical initialization of an atmospheric model, which should lead to much more accurate low-latitude forecasts. This is very important for tropical cyclone prediction. The Office of Naval Research-sponsored success story of Professor O'Brien illustrates a newly discovered El Niño teleconnection between the tropical Pacific and eddy generation along the Alaskan coast.*

Dr. Joseph W. McCaffrey, Jr.
Naval Research Laboratory
Stennis Space Center, MS
CTA Leader for CWO

# First Pacific Ocean Model with 1/16-Degree Resolution

H.E. Hurlburt and E.J. Metzger
*Naval Research Laboratory, Stennis Space Center, MS*
A.J. Wallcraft
*Planning Systems Inc., Slidell, LA*

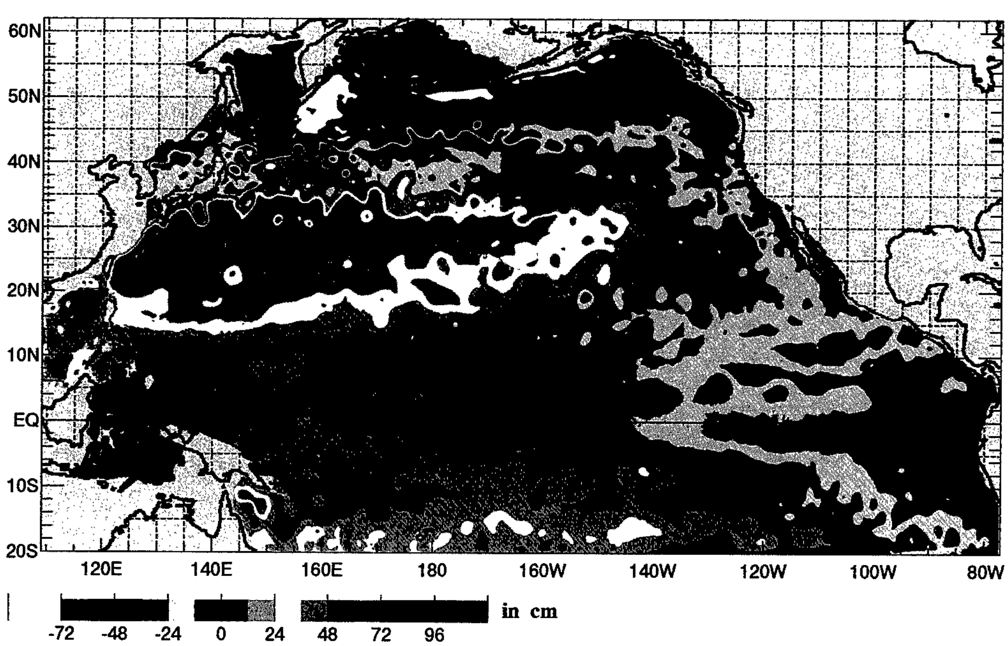
***Computer Resources:*** Cray C916 [NAVOCEANO MSRC] and Cray Y-MP M98 [DNA/LANL DC]

***Research Objectives:*** To develop an eddy-resolving global and basin-scale ocean model and prediction system. This includes understanding of ocean dynamics, model validation, naval and global change applications, oceanic predictability, and observing system simulation.

***Methodology:*** The NRL Layered Ocean Model is typically tens to hundreds of times more efficient than other ocean models in computer time/model year. This is primarily because Lagrangian layers are used in the vertical, and a semi-implicit time scheme makes the time steps independent of all gravity waves. We have developed a scalable portable version of the model that can run on any HPC system configured for large applications.

***Results:*** The world's first 1/16-degree Pacific Ocean model (north of 20 degrees south) gives widespread improvements over 1/8-degree resolution on the large scale as well as the mesoscale. Improvements include sharper definition and greater eastward penetration of the basin-wide subarctic and Kuroshio Extension fronts. The model was spun up from rest, driven by monthly climatological winds at lower resolution for 155 years, and has run 46 years at 1/16 degrees, including 2 interannual simulations forced from 1981 by daily winds from the European Centre for Medium-Range Weather Forecasts.

***Significance:*** We are discovering the widespread importance of mesoscale flow instabilities in allowing bottom topography to steer upper ocean currents. This upper ocean-topographic coupling requires that mesoscale eddies be very well resolved to obtain sufficient coupling. Thus, this fundamental and major topographic effect is largely missed at coarser resolution. Eddy-resolving global and basin-scale ocean modeling is a Grand Challenge problem. By a careful choice of algorithms we have run such a model on existing supercomputers. Eddy-resolving ocean models are an important milestone toward a global ocean monitoring and prediction system. Applications include ship routing; search and rescue; antisubmarine warfare; environmental simulation; ocean observing system simulation; and inputs to coastal, ice, and weather models.




*Sea surface height snapshot for 21 January 1986 simulated by a Pacific Ocean model with 1/16-degree resolution for each variable. Contour interval is 12 cm.*

# Convective Rainfall Initialization

A.H. Van Tuyl and G.D. Rohaly
*Naval Research Laboratory, Monterey, CA*

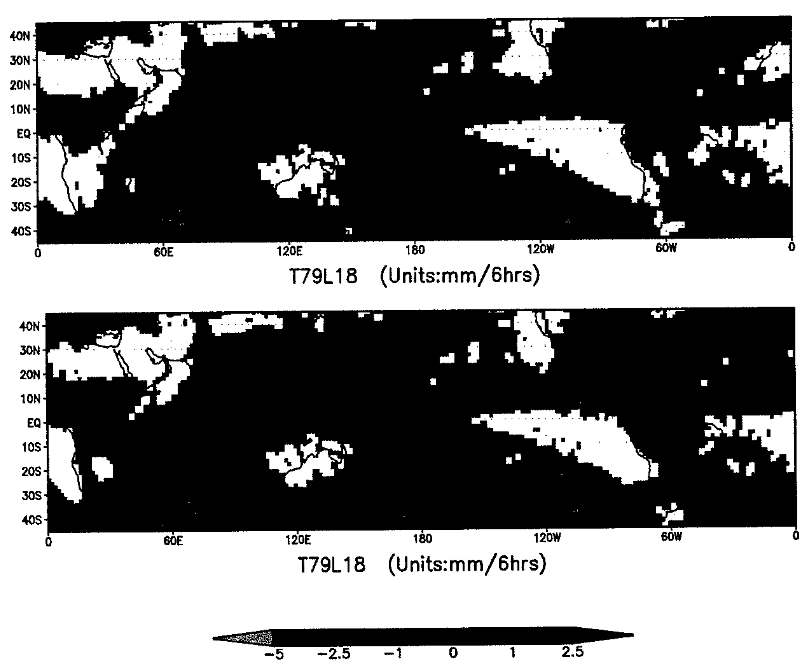
***Computer Resources:*** Cray C916 [CEWES MSRC and NAVOCEANO MSRC] and Cray Y-MP [CEWES MSRC and NAVOCEANO MSRC]

***Research Objectives:*** To implement a scheme of physical initialization in the Navy Operational Global Atmospheric Prediction System (NOGAPS) and to evaluate its success. The scheme consists of matching observed and model-produced diabatic quantities, most notably convective rainfall, prior to the start of a prediction run. Success is measured both by the closeness of this matching and by the degree of improvement in the ensuing forecast.

***Methodology:*** An estimate of convective rainfall is obtained from satellite microwave data, either SSM/I or MSU. The NOGAPS model is then integrated for a specified period during which the model rain is matched (to the extent possible) to the time-interpolated observed rainfall rate. This matching is performed at each model time step by adjusting the model's moisture field. Specifically, a perturbation in relative humidity, linear in pressure, is added to the model relative humidity. A bisection technique is used to help achieve the closest possible matching. Four iterations per time step are generally sufficient.

***Results:*** The physical initialization produces very good agreement between observed and model-generated rainfall during assimilation, with spatial correlations as high as 0.97 for 24-hour convective accumulations. Rainfall maxima, for example those associated with tropical cyclones, can be matched extremely well using physical initialization, even when these features are entirely absent from a control run. A somewhat lesser positive impact is seen in forecasts begun from the assimilated states, with noticeable improvement out to at least 24 hours. This indicates that a model circulation capable of supporting the observed rainfall has been developed (at least partially) through the assimilation.

***Significance:*** This physical initialization technique allows the use of rainfall data in tropical regions, where convective forcing is dominant and little additional data are available. Forecasting skill, therefore, should improve by the use of these data. Tropical cyclones, which are of particular interest to the Navy, should be among the low-latitude phenomena whose prediction is most greatly enhanced by physical initialization. In addition, because this method is being applied to the NOGAPS global model, improvement may extend to midlatitude forecasts as well as those in the tropics.




*Time-averaged difference between 6-hour NOGAPS convective rainfall accumulation and the observed accumulation (top) without physical initialization, (bottom) with physical initialization. Time average is over the entire assimilation period (23 August 1993—6 September 1993). The NOGAPS stable precipitation is not included.*

# Improved Prediction of Cloud Cover

T.N. Krishnamurti
*Florida State University, Tallahassee, FL*
*Air Force Office of Scientific Research, Washington, DC*

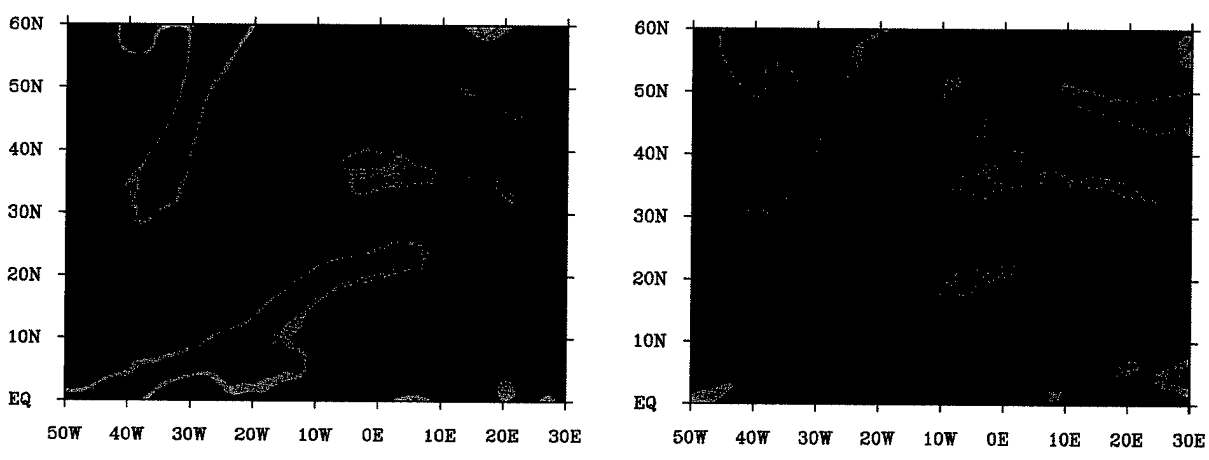
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC]

***Research Objective:*** The interests of the U.S. Air Force and of general aviation require a high-precision forecast of cloud cover within a short-range (24 to 48 hour) forecast. The requirements for medium-range (6 to 8 days) forecasts are considerably less stringent. We have developed an improved cloud prediction procedure within a high-resolution global model.

***Methodology:*** The cloud cover prediction procedure involves five steps and builds on our successful "physical initialization" scheme: (1) Observed rain rates, inferred from Air Force DMSP satellites (e.g., SSM/I microwave instruments), are assimilated in the model via a reverse cumulus parameterization algorithm. (2) Surface fluxes are made consistent with prescribed rain via a reverse similarity algorithm. (3) Model-based outgoing longwave radiation (OLR) is matched to satellite OLR using a bisection method, which modifies the vertical distribution of humidity. (4) Cloud cover is initialized by modifying threshold relative humidity—matching observed cloud from Air Force RTNEPH data with model-produced cloud by using iterative algorithms. (5) Assimilate the rain rate, OLR, and cloud fractions within the global model by using a Newtonian relaxation scheme.

***Results:*** The figure shows that such an assimilation has a strong positive impact on the prediction of cloud cover. The example shows the cloud cover associated with a trough off West Africa. The trough is visible only in the left panel forecast, which used the physical initialization procedure.

***Significance:*** The physical initialization procedure provides a major improvement in the initialization of cloud fractions, OLR, rainfall, and surface fluxes.




*Total cloud from 24-hour prediction beginning January 24, 1991, 1200Z, with (left panel) and without (right panel) physical initialization*

# Numerical Weather Prediction of Cloud Liquid Water

G.D. Modica
*Phillips Laboratory, Hanscom Air Force Base, MA*

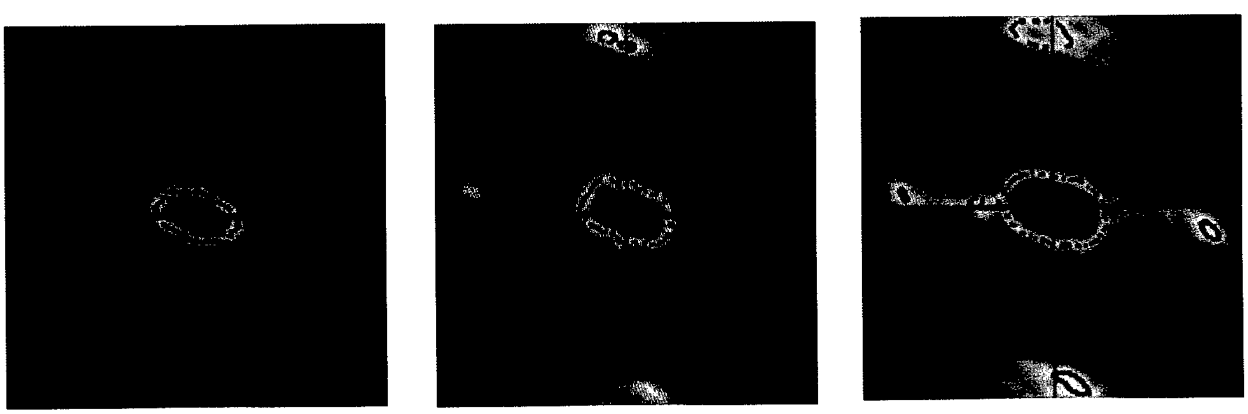
***Computer Resource:*** Cray C916 [CEWES MSRC and NAVOCEANO MSRC]

***Research Objective:*** To assess the sensitivity of cloud liquid water (CLW) forecasts to changes in the spatial resolution of the numerical weather prediction (NWP) model.

***Methodology:*** A regional NWP model that included a bulk microphysics representation of precipitation processes was configured with four different computational grids: Ds = 100 km, 18 vertical levels; Ds = 100 km, 36 levels; Ds = 50 km, 18 levels; and Ds = 50 km, 36 levels. The experiments were originally performed for the Comparison of Mesoscale Prediction and Research Experiment (COMPARE), which was intended to measure differences/similarities among forecasts from several mesoscale NWP models when started from the same initial conditions. The meteorological case was one of explosive cyclogenesis over the western Atlantic during winter. The last experiment (Ds=50 km, 36 levels) was taken to be the control, and cloud forecasts from it were compared first to those with half the horizontal resolution (experiment 2), and then with half the vertical resolution (experiment 3). Cross correlation fields were computed to provide information on both phase and amplitude differences.

***Results:*** CLW distributions from forecasts up to 36 hours at several constant pressure levels from the model were compared to the control. Some results for the 36-hour forecast at 850 hPa are shown in the figure. Since the middle panel (exp4 o exp3) correlates better with the autocorrelation field (left panel, exp4 o exp4) than does the right panel (exp4 o exp2), the conclusion is that diminishing the horizontal resolution by half results in a poorer CLW forecast than when halving the vertical resolution. The same panels from 6 hours into the forecast (not shown) reveal very little variation among the experiments. This suggests that the spatial resolution issue is less important during the earlier stage of the integration. There is also little variation among the experiments at mid-tropospheric levels.

***Significance:*** Clouds and precipitation can significantly impact Air Force operations and systems. For example, clouds can obscure targets and precipitation can affect microwave communication. If cloud forecasts from NWP models can be improved significantly, the effect will be one of force multiplication, because combat resources would not be wasted on failed missions caused by poor line-of-site visibility. Pilot safety, E/O weapon performance, and communications will also be improved. Better predictions of clouds, precipitation, and associated aviation-impact variables (e.g., icing, downbursts) are relevant to the civilian aviation community and other general interests affected by the weather.



*Correlation fields of CLW for 36-hour forecast at 850 hPa. Left panel shows autocorrelation of CLW (exp4 o exp4); middle panel for exp4 o exp3; right panel for exp4 o exp2. Red shades indicate values close to 1; black color for values close to –1.*

# Recent Variations of Arctic Ice Cover

S.A. Piacsek, R. Allard, and P. Jayakumar
*Naval Research Laboratory, Stennis Space Center, MS*

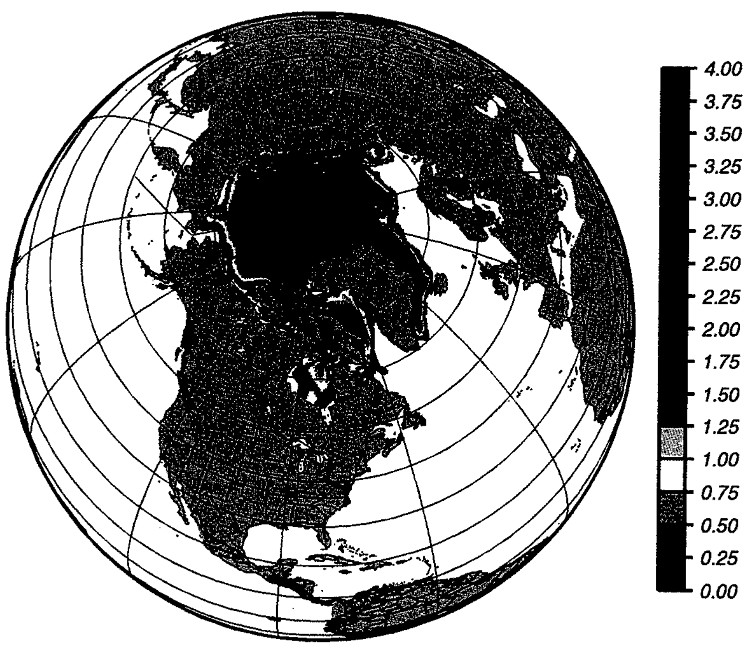
***Computer Resource:*** Cray C916 [NAVOCEANO MSRC and CEWES MSRC]

**Research Objectives:** To understand and simulate the synoptic, seasonal, and interannual variations in the Arctic ice-ocean system. Particular processes include: decadal variations in the Arctic; the effects of different atmospheric and radiation forcings; the effect of Arctic river discharges; and the process of deep-water mass formation.

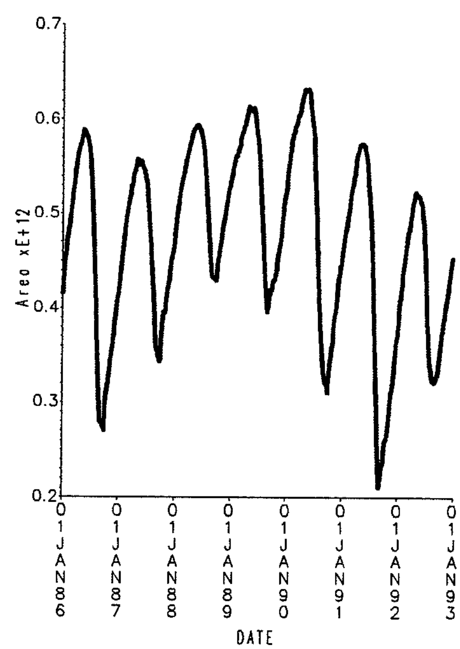
***Methodology:*** Finite-difference formulations of the momentum, heat, salt, and ice transport equations are solved on HPC computers. The matrix resulting from implicit treatment of the ice rheology equations is solved by a four-color successive over-relaxation (SOR) algorithm, which is both vectorizable and parallelizable. The ocean code is fourth-order accurate in the pressure, advection, and Coriolis terms, and can operate with an order of magnitude smaller numerical friction than previous codes.

***Results:*** We have finished a 7-year simulation for the period 1986-1992. A trend of diminishing winter ice volume but not ice-covered area was found since 1990, with no clear overall trend for the summer minima. These trends (except for 1991) have recently been verified by remotely sensed SSMI data.

***Significance:*** The presence of ice can interfere with Navy and commercial shipping in the northern seas. Ice is a major impediment to exploration off the North Shore of Alaska, and to fishing in the Gulf of Alaska and the Labrador Sea. The Arctic ice cover is an important component of the Earth's climate system, one that will be the first affected, and therefore a good indicator, of potential global warming.




*Simulated Arctic ice thickness (meters) for June 30, 1992*




*Total Arctic ice volume changes between 1986-1992 ($10^{12}$ $m^3$)*

# Interannual Variability Along the Coast of Alaska Induced by Teleconnection from the Tropical Pacific Ocean

J.J. O'Brien
*Florida State University, Tallahassee, FL*
*Office of Naval Research, Arlington, VA*

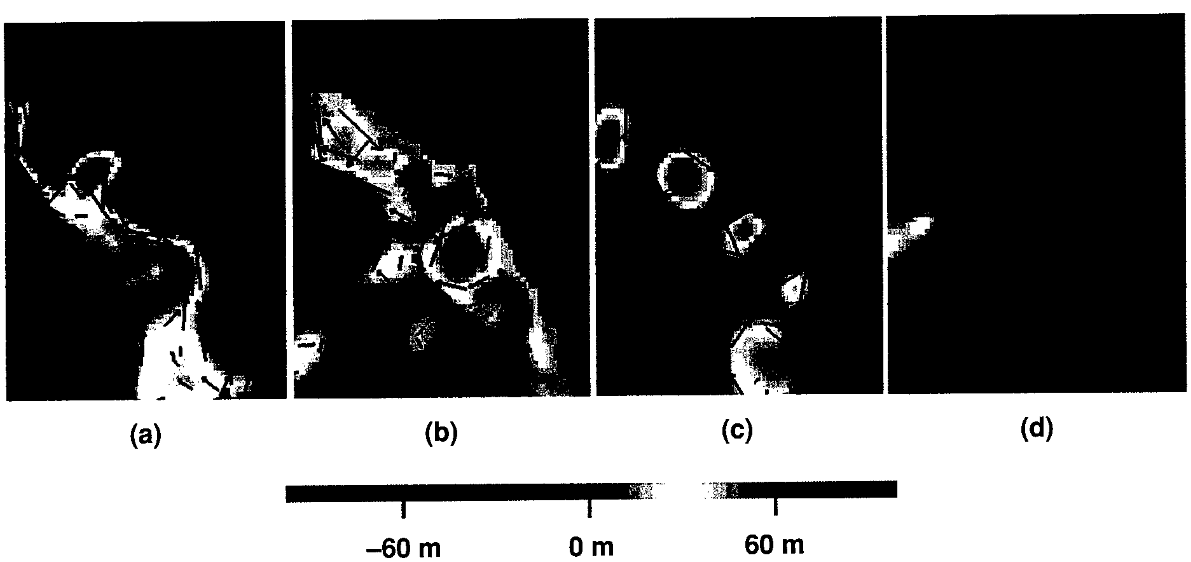
***Computer Resource:*** Cray Y-MP [NAVOCEANO MSRC]

***Research Objective:*** To investigate the high-latitude impact of coastal Kelvin waves generated during the extremes of the El Niño-Southern Oscillation (ENSO).

***Methodology:*** The Naval Research Laboratory (NRL) high-resolution, multilayer Pacific ocean model is driven by a modified version of the ECMWF (European Centre for Medium-Range Forecasting) surface winds corresponding to 1981-1994. This is a cooperative effort, with the computations done by the ocean modeling team at NRL and the output analysis done by scientists at Florida State University.

***Results:*** Downwelling Kelvin waves originating in the equatorial Pacific ocean can enhance the vertical shear in the Gulf of Alaska, destabilize the mean coastal currents in the region, and form long-lived baroclinic eddies. Upwelling waves stabilize the current system. The model accurately reproduces much of the observed variability in the region of interest, as demonstrated by model comparisons with coastal sea-level stations and observations of eddy activity. ENSO is the dominant source of interannual variability along the coast of the Gulf of Alaska.

***Significance:*** This successful project was conducted as a cooperative effort between Naval and academic personnel. Major changes in the coastal circulation in the Gulf of Alaska are shown to be related to El Niño events in the tropical Pacific Ocean. These changes have a major impact on submarine operational security and civilian fisheries.




*The ocean circulation in the model for the same day (February 28) of four different years: (a) 1983, (b) 1986, (c) 1988, and (d) 1989. Both (a) and (c) follow El Niño events; (d) follows an El Viejo event. The anticylonic circulation in (d) is a remnant of the eddies generated the year before. The domain of each image is between (53°N, 144.25°W) and (61.25°N, 131.75°W). Colors indicate deviation from the mean thickness of the upper two layers; arrows depict the direction and strength of the currents.*

# Logistics-Over-The-Shore Wave Hindcasting

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*Army Engineer Waterways Experiment Station, Vicksburg, MS*

***Computer Resource:*** Cray C916 [CEWES MSRC]

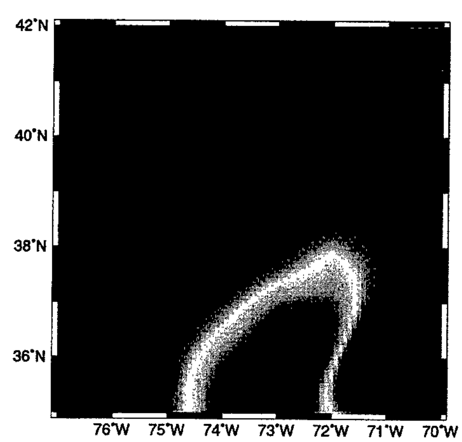
***Research Objective:*** To develop, test, and implement state-of-the-art spectrally based wave models for the simulation of deep, intermediate, and nearshore wave conditions for Logistics-Over-The-Shore (LOTS) applications.

***Methodology:*** LOTS operations are performed in the nearshore region, less than 5 km from shore. Accurate wave estimates for these operations are critical to operation success. These regions are extremely small compared to global-scale water bodies. However, what is generated from the far wave field (principally from oceanic conditions) will have a significant impact on the nearshore area. With a nested grid approach, bathymetry, geography (shoreline/islands), and meteorological conditions must be resolved in each gridded area. The Army Engineer Waterways Experiment Station (CEWES) has cooperated in research initiatives with various internationally recognized spectral wave modelers to develop, test, and implement technologies in marine applications. The 3GWAM model has been used in deep and intermediate waters. In shallow water, solutions to the various source/sink terms break down, and alternate solution methods are required. One such wave model, STWAVE, recently developed and modified at CEWES, can accurately estimate the extreme nearshore wave climate, even in areas of highly variable bathymetric features.

***Results:*** Oceanic grids require resolution on the order of 60 km (typically a mesh of more than 100,000 cells); shelf-area grids are resolved to 15 km or less; nearshore grids must accurately describe the fine-scale bathymetric and geographical features with a mesh size on the order of 1-5 km. Initial results indicate that present wave modeling technologies provide a relatively good degree of accuracy. However, tolerances required for operations fall below the tolerance of ±40 cm presently provided by these technologies. Thus, further research is being performed to increase the accuracy of the wave models.

***Significance:*** Accurate historical wave climatologies are part of the environmental information required for successful LOTS operations. With present state-of-the-art modeling tools, this can be achieved quite well in most situations.


*Wave height color contour (meters) for October 26, 1990 (2100 GMT) storm, shelf-scale region*




*Wave height color contours for refined grid of coastal region*

# Coastal and Semi-Enclosed Seas/Tactical Scale Modeling

A.L. Perkins, L.F. Smedstad, and G.W. Heburn
*Naval Research Laboratory, Stennis Space Center, MS*

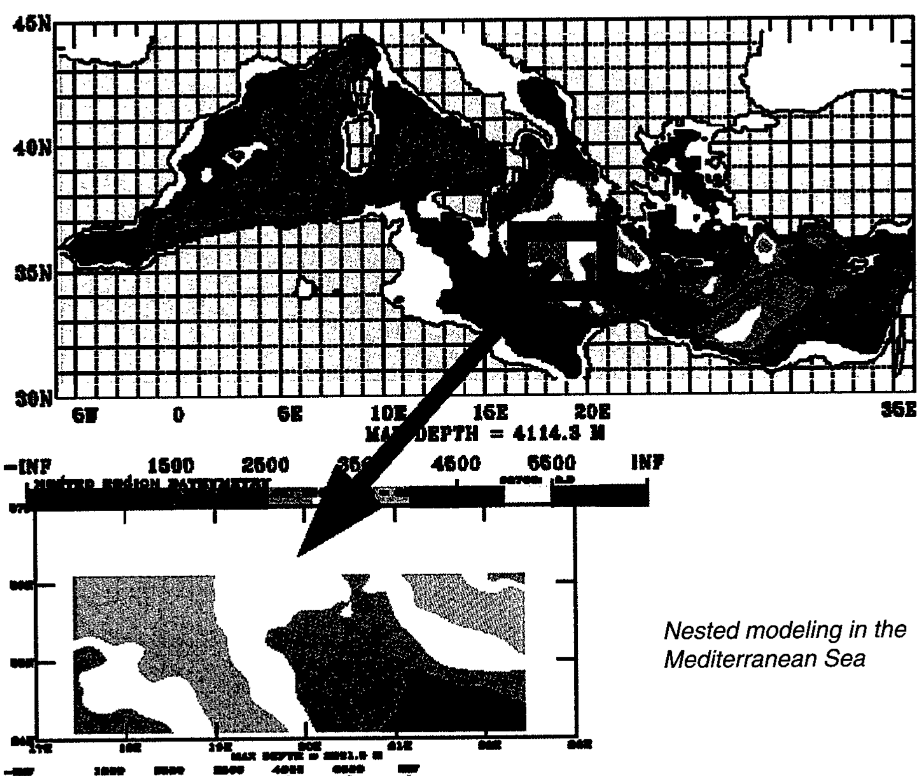
***Computer Resource:*** Cray Y-MP [CEWES MSRC] and Cray C90 [NAVOCEANO MSRC]

***Research Objectives:*** To increase our understanding of the oceanography on Navy-priority, enclosed and coastal seas and to develop, demonstrate, and transition nowcast and forecast systems for these areas. This project develops, implements, and evaluates ocean models and prediction systems of semi-enclosed and shallow coastal seas.

***Methodology:*** Develop and test nesting techniques within the Mediterranean Sea using the NRL Layered Model. Use the resulting nested ocean model to study predictability and sensitivity to forcing between deep and shallow coastal regions. Numerical experiments and model/data comparisons will be used to examine sensitivity to external factors. Model results will be used to create a testbed for future coupled modeling efforts.

***Results:*** The Mediterranean model has been adapted to use NORAPS forcing (needed for operational forecasting). Model sensitivity studies using both the NRL hydrodynamic and thermodynamic models have been conducted for the Mediterranean basin. Several refined nested experiments have been performed in the Ionian Basin of the Mediterranean. Model robustness has also been tested with nested experiments.

***Significance:*** Navy coastal operations require environmental knowledge analogous to open-ocean requirements. Historically, the Navy has fought in coastal waters more often than in the open ocean (this is also the recent experience, from World War II to the present). An improved understanding and ability to predict coastal processes will directly bear on issues such as amphibious warfare, shallow-water acoustic and nonacoustic antisubmarine warfare, mine and countermine warfare, search and rescue, and special warfare.




*Nested modeling in the Mediterranean Sea*

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### Recent Variations of Arctic Ice Cover

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### Coastal and Semi-Enclosed Seas/Tactical Scale Modeling

G.W. Heburn, L.F. Smedstad, and M.M. Hines, "The Dynamics of the Seasonal Variability of the Ionian Sea," presented at IAPSO XXI General Assembly, 8 August 1995.

# Signal/Image Processing

*Signal and image processing (SIP) techniques are used throughout DoD to extract useful information, such as target detection, tracking, and identification, from raw sensor signals. Signal and image processing span from the development and simulation of new concepts, to their real-time implementation on ruggedized systems suitable for field deployment. The rapid advance of embedded HPC technology allows low cost, scalable, programmable systems to replace the expensive point solutions previously required to meet the needs of high performance military systems.*

*The first two success stories apply HPC technology to the challenging problem of clutter and jammer suppression on advanced airborne radar platforms using Space-Time Adaptive Processing. The third success uses HPC resources to form high-resolution synthetic aperture radar images and recognize targets. HPC technology also plays a critical role during the development and simulation of new signal processing concepts, leading to their deployment in systems. The fourth success story uses HPC to evaluate closed-loop control algorithms for adaptive deformable mirrors for large optics. The fifth success story uses the power of HPC to simulate the validity of new sea clutter models to improve a radar's ability to see small targets buried in clutter returns.*

*The final success story searches the sky for new pulsars, collapsed stars that provide accurate timing references, by examining signals from the large-aperture radio observatory at Arecibo, Puerto Rico.*

Dr. Richard W. Linderman
Rome Laboratory
Griffiss AFB, NY
CTA Leader for SIP

# Scalable High-Performance Computing for STAP

J.R. Samson, Jr. , D.A. Grimm, K.K. Morrill, and T.J. Andresen
*Honeywell Inc., Clearwater, FL*
*Rome Laboratory, Griffiss AFB, NY*

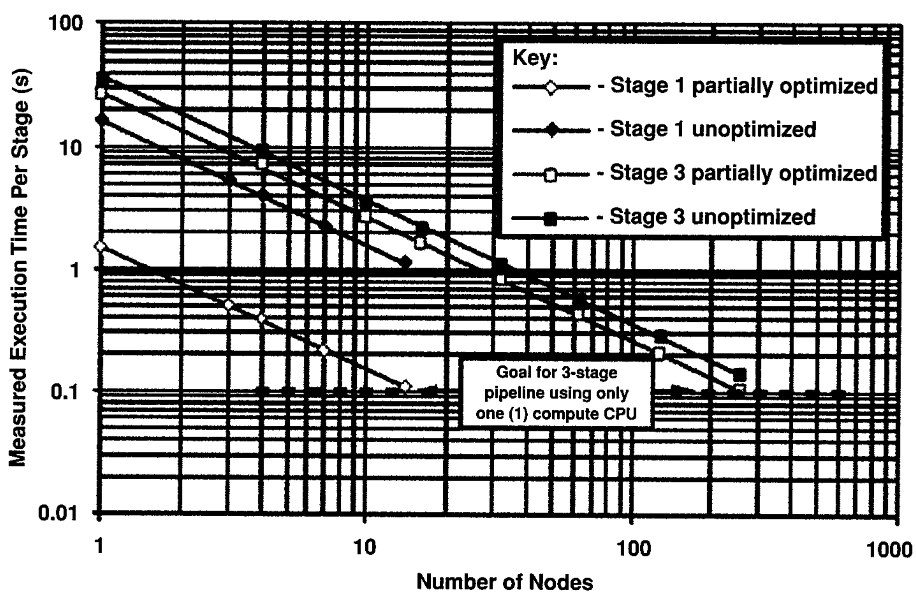
***Computer Resource:*** Intel Paragon [RL DC]

**Research Objective:** To demonstrate the efficacy of a high-level, data parallel, data flow approach to scalable STAP (Space-Time Adaptive Processing) on a general-purpose, massively parallel, high performance computing system.

***Methodology:*** All of the benchmarks were implemented with a high-level, data parallel, data flow approach using Honeywell's Configurator and Data Flow Shell. These tools were developed to augment the software tools available with the commercial Paragon system. A pipeline implementation was chosen to support low end-to-end latency and high sustained throughput with the overlap of processing and communication to mask communication overhead to the maximum possible extent.

***Results:*** The efficacy of the high-level, pipelined data flow implementation and the inherent scalability of five STAP benchmarks on processing configurations ranging from 8 nodes to more than 300 nodes were demonstrated. All five pipelined benchmarks demonstrated measured, sustained, high overall implementation efficiency (34 - 69%), high relative speedup [the ratio of speedup to the number of compute nodes used (0.69 - 0.91)], and high compute resource utilization efficiency (81 - 91%) depending on the benchmark. The Configurator and Data Flow Shell tools were shown to be very powerful aids for automatic, scalable parallelization of sequential C code. They demonstrated high software parallelization productivity, while requiring no application software tweaking or modification to change the processing configuration. In addition, high software reuse and the benefits of various optimization techniques, including the use of existing, highly optimized libraries, were demonstrated.

***Significance:*** Heretofore, it had been concluded by many that fine-grained systolic implementations were the only solution to the STAP problem. This research showed that (1) the Paragon/Touchstone high performance mesh communication fabric is well-suited for a high-level data parallel, data flow implementation, (2) a high performance, cost-effective implementation is possible with this high-level data flow approach, (3) high implementation efficiencies can be attained, (4) STAP latency requirements can be met, and (5) the Paragon/Touchstone design is scalable with the size of the STAP problem. These results are applicable to many other signal processing domains implemented on a Paragon/Touchstone high performance computing system.



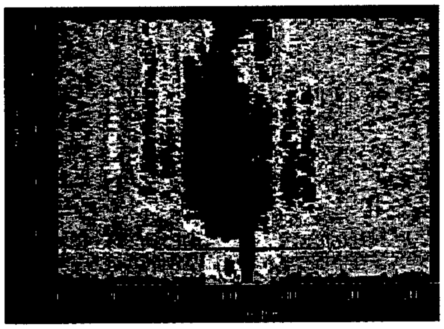

*Demonstrated scalability performance for STAP APT benchmark [unoptimized (100% original C-code) and partially optimized (for example, high-performance, reusable libraries)]*

# Embedded HPC for Real-Time Airborne STAP Radar Experiment

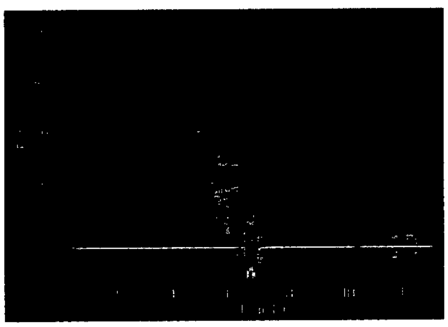
R.W. Linderman, M.H. Linderman, and R.D. Brown
*Rome Laboratory, Griffiss AFB, NY*

***Computer Resource:*** Intel Paragon [RL DC]

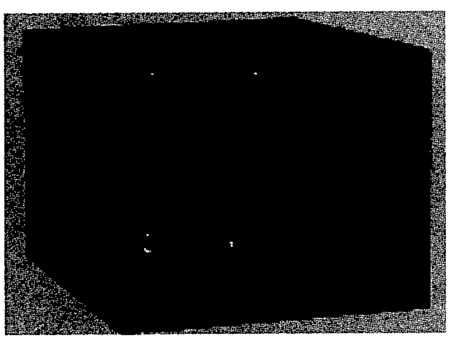
***Research Objective:*** To demonstrate that advanced Space-Time Adaptive Processing (STAP) algorithms can be computed in real time onboard aircraft with multichannel, phased array radars and meet the size, weight, and power constraints by using HPC technology in an embedded form.



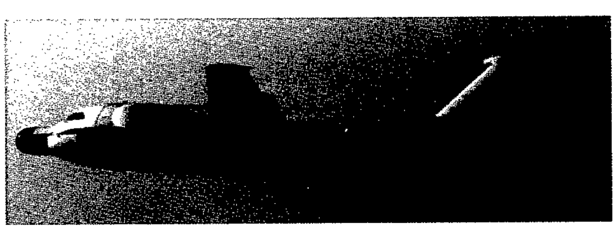
*Clutter prior to STAP*



*After STAP processing*



*19-in. ruggedized rack*



*BAC 1-11 with phased array*

***Methodology:*** The STAP algorithms were implemented and optimized to meet the real-time constraints. Prerecorded data, available from previous test flights of the BAC 1-11 aircraft with its sidemounted, 24-channel, L-band phased array radar, was fed across a high performance parallel interconnect (HiPPI) at real-time rates to emulate the sensor inputs. A subset of 25 of the 321 nodes on the Paragon at the Rome Laboratory was used to perform the real-time calculations. The number of nodes was limited by a requirement that the system draw less than 20 amps at 110 volts while onboard the aircraft. The application was then ported to 25 Paragon nodes in two standard 19-inch ruggedized racks to meet the aircraft's size and weight constraints. These nodes allowed a peak throughput of 7.5 billion floating point operations per second (Gflops). The approach allowed these nodes to be used in a flexible programming environment while delivering a high percentage of peak performance.

***Results:*** Both the OSF and SUNMOS operating systems were considered for this experiment. SUNMOS was chosen because it had less overhead, faster message passing, better single-processor performance (because of the larger 4 MB page size), and allowed access to all three of the processors on each node (OSF granted access to only two). A simple post-Doppler adaptive beamforming version of STAP was implemented first, requiring about 1.5 Gflops of sustained performance. The more aggressive PRI-staggered post-Doppler algorithm, requiring 4.5 Gflops of sustained (60% of peak) performance, was then implemented and optimized. In both cases, the Paragon nodes took raw channel returns as input and performed all the steps required to generate target detections as output for display on an attached workstation.

***Significance:*** Some researchers wonder whether HPC technology can meet the size, weight, power, and real-time throughput and latency requirements of embedded signal processing applications. This success demonstrates that it can be done, even for very challenging radar applications. HPC architectures can be ruggedized for embedded environments and still deliver 60% of the advertised "peak" throughput under real-time constraints while concurrently providing scalability and flexibility superior to that of traditional approaches that use application-specific integrated circuits or commercial digital signal processing boards.

# ASARS II Image Formation and ATR on a General-Purpose MPP Testbed

C. Hendrickson and D. Cottel
*Naval Command, Control and Ocean Surveillance Center, San Diego, CA*

***Computer Resource:*** Intel Paragon [NCCOSC DC]

***Research Objective:*** Current operational synthetic aperture radar (SAR) systems provide real-time processing of raw radar data into two-dimensional focused images, but lack the flexibility to enhance the algorithms and to scale for increased processing performance. Automatic Target Recognition (ATR) algorithms are currently not operational due in part to real-time processing requirements. The general objective of this effort was to provide an image formation and ATR HPC testbed for algorithm enhancements, limited production, and real-time demonstrations. Specifically, the objective was to port Advanced Synthetic Aperture Radar System II (ASARS II), one of the more advanced systems aboard the U2 aircraft, and ATR algorithms to the Intel Paragon to demonstrate the feasibility of real-time processing of operational SAR systems on a general-purpose massively parallel processor (MPP).

***Methodology:*** The Intel Paragon at NCCOSC was selected because of its clearance for processing classified imagery and its availability to the contributing organizations. The parallel software development tools developed as a result of DoD HPC investment were also used to facilitate the implementation of algorithms on the Paragon in a parallel pipeline fashion. Hughes Aircraft had developed a real-time ASARS II processor using special purpose hardware and software. NRaD worked with Hughes to port their processor to the Paragon in a high-level language. The Massachusetts Institute of Technology/ Lincoln Laboratory (MIT/LL) had developed ATR algorithms for their Advanced Detection Technology Sensor. MIT/LL ATR algorithms were modified for ASARS II, transitioned to NRaD, and then implemented by NRaD on the Paragon. Display tools were also required to view the SAR imagery and the resulting detected and identified targets.

***Results:*** Hughes' ASARS II image formation, MIT/LL's ATR, and NRaD's display were successfully integrated and ported to the Intel Paragon. The results demonstrated the feasibility of real-time processing of an operational SAR system on a general-purpose MPP.

***Significance:*** A general-purpose MPP testbed provides military and commercial SAR systems with the flexibility for algorithm enhancements, production capabilities, real-time demonstrations, and portability to other HPC architectures.

*U2 aircraft housing the ASARS II*

# Leading-edge Methods in Atmospheric Imaging

B.L. Ellerbroek
*Phillips Laboratory, Kirtland AFB, NM*
R.J. Plemmons
*Wake Forest University, Winston-Salem, NC*
*Air Force Office of Scientific Research, Washington, DC*

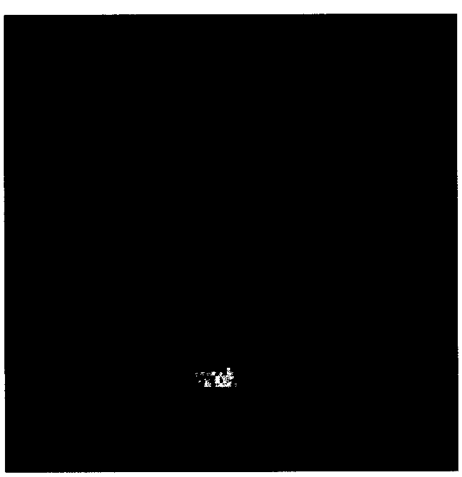
***Computer Resource:*** IBM SP2 [MHPCC DC]

***Research Objective:*** To develop rigorous mathematical models, algorithms, and supercomputer implementations for adaptive optics and image postprocessing, with applications to imaging through the atmosphere.

***Methodology:*** The research concerns two major projects in atmospheric imaging. The first involves adaptive deformable mirror control. Deformable mirrors operating in a closed-loop adaptive optics system can partially compensate for the effects of atmospheric turbulence, using either a natural guide star (point) image or a guide star artificially generated from the backscatter of a laser-generated beacon. This optimal control system is being designed in conjunction with the DoD's largest optical telescope facility located at Phillips Laboratory in New Mexico (PLK). The massively parallel IBM SP2 at the MHPCC is being used for simulation experiments. The second project concerns nonlinear iterative methods for large-scale image postprocessing computations, using a priori knowledge about the degradation phenomena, in this case atmospheric turbulence. Our parallel codes running on the SP2 can handle large-scale restorations of Air Force data with considerable savings in computation time.

***Results:*** One successful project concerns new multiple bandwidth approaches to deformable mirror control for compensation of the effects of atmospheric blurring on ground-to-air, air-to-air, and air-to-ground imaging. The authors have helped to develop a theory for multiple-bandwidth, closed-loop, adaptive control methods to adjust the shape of these mirrors in real time, and have shown the advantages of a class of new parallel fast Fourier transform-based nonlinear postprocessing reconstructions. Computations on the IBM SP2 have shown the practical advantages of these methods. The figure below illustrates these reconstructions using real data obtained at PLK.

***Significance:*** In addition to the DoD work described above, applications to civilian technology include astronomical and medical imaging as well as remote sensing for commercial purposes. In astronomical imaging, there is technology transfer to the Gemini 8-meter telescope international project. Biomedical applications include the use of low-energy laser beacons as an aid in deblurring images of the retina through the eyeball. The new postprocessing methods can also be applied to enhancing remote sensing images of the Earth for agriculture, law enforcement, and geophysics.



*Satellite image reconstruction: Uncompensated image (left) and on-line compensation by adaptive optics, with postprocessing on the 400-node SP2 at the MHPCC (right).*

# Statistical Modeling of Radar Sea Clutter

D.W. Stein and B.F. Summers
*Naval Command Control and Ocean Surveillance Center, San Diego, CA*

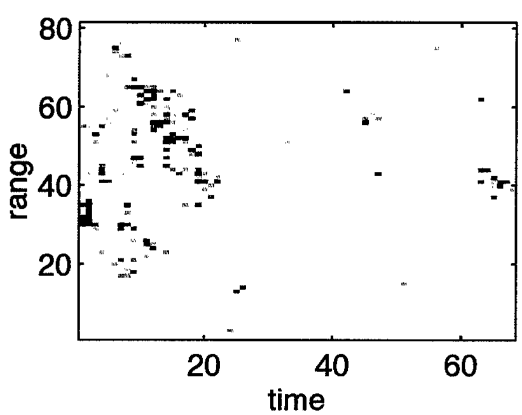
***Computer Resource:*** Convex SPP-1 [NCCOSC DC]

Research Objective: The detection of targets on the surface of the sea using high-resolution radar is often hampered by sea spikes, such as those evidenced in the sea clutter image below. Using limited data sets, we have found that exponential mixture densities may provide a useful statistical model of high-resolution sea clutter intensity. The purpose of this project is to determine empirically the applicability of this model to a larger set of such data.

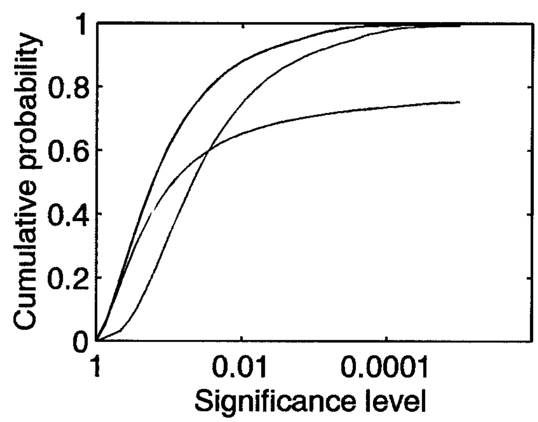
***Methodology:*** High-resolution, low-pulse-rate sea clutter data were collected at NCCOSC. Five hundred thousand 1-second time series of 60 pulse-per-second data from fixed range bins were fit to exponential and two and three state exponential mixture densities using the expectation and maximization algorithm. Goodness-of-fit statistics were then calculated for each model. The code was implemented on the Convex SPP-1 by distributing time series to the processors. The processors then independently estimated model parameters and calculated goodness-of-fit statistics. These values were then saved in global memory.

***Results:*** The applicability of a class of densities to a collection of time series was assessed using the cumulative distribution of the significance level of the goodness-of-fit statistic comparing the density of each time series to the best fitting representative of the class of densities. These distributions, obtained using one-fourth of the data evaluated, are shown in the figure below for the one (red), two (yellow), and three (green) state exponential mixture models. The cumulative distribution of the maximum of the significance levels of these models is shown in blue. The figure shows that approximately 70 percent of the time series had an exponential density significance level above 0.001, and approximately 95 percent of the time series had either the one, two, or three state exponential mixture density significance level above 0.001.

***Significance:*** These results show that exponential mixture densities are applicable to the low-pulse-rate sea clutter intensity data. Therefore, target detection in this environment should be significantly enhanced by using algorithms based on this model.




*Sea clutter*




*Goodness-of-fit of 125,000 time series*

# High-Performance Techniques for the Detection of Weak Signals

R.S. Foster
*Naval Research Laboratory, Washington, DC*

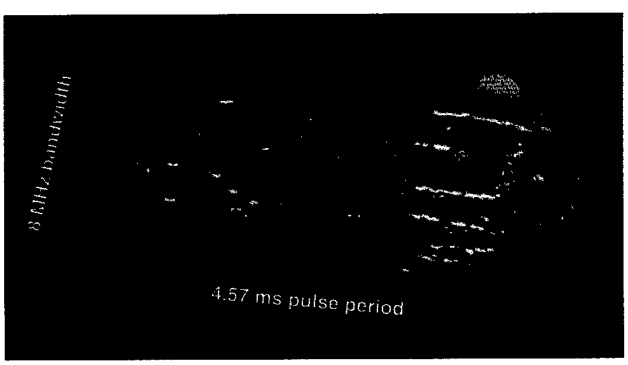
***Computer Resource:*** SGI Power Challenge [ARL MSRC] and IBM SP2 [MHPCC DC]

***Research Objectives:*** To develop a parallel search code in a scalable computing environment to process very large data sets as part of a basic research program studying pulsar astrophysics. Pulsars are degenerate stars that have collapsed under their own gravity and rapidly rotate, thereby emitting pulsed radiation. To achieve an understanding of the absolute precision of pulsar timing, we are investigating the physical processes of pulsar formation, emission, and evolution in order to determine whether (and how) pulsars can provide a space-time reference frame.

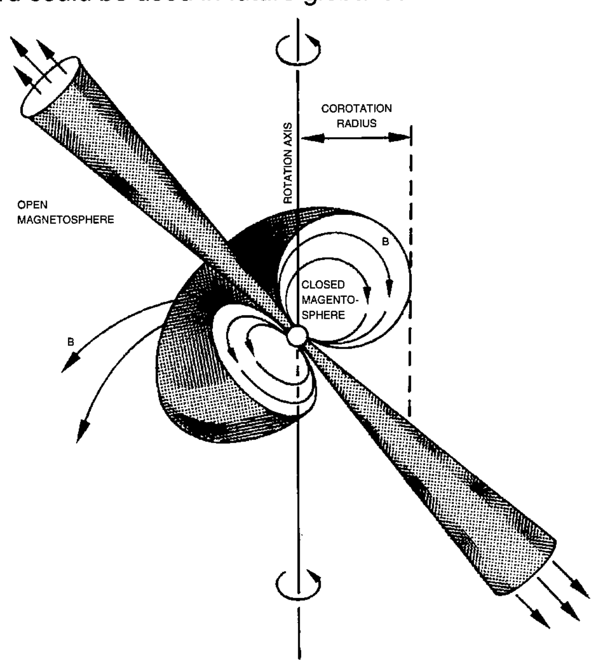
***Methodology:*** The computational task needed to detect millisecond pulsars involves searching for weak chirped signals embedded in large, two-dimensional frequency-time data sets. The search process requires detecting signals in a parameter space, that is, at minimum, three dimensions: dispersion measure, rotational period, and pulse duty cycle or shape. The numerical techniques use fast Fourier transforms and harmonic folding to discover signals above a certain threshold.

***Results:*** Four new millisecond pulsars have been discovered using DoD computational assets. All of the data were collected at the National Astronomy and Ionosphere Center in Arecibo, Puerto Rico. One of the detected millisecond pulsars now appears to be the most stable natural clock on time scales longer than six months.

***Significance:*** Increasing the number of known pulsars will improve our knowledge of the evolutionary characteristics of these stars. A small number of millisecond pulsars distributed around the sky could be used to stabilize the International Atomic Time on time scales longer than six months; this is not presently feasible with current atomic clocks. It thus addresses a specific need of the U.S. Naval Observatory's Congressionally mandated requirement to maintain national standards for precise time and time interval measurements and navigation. A stabilized time standard could be used in future global communication and solar system navigation applications.




*Two-dimensional pulsar phase-frequency plane of a newly detected millisecond pulsar, PSR J1713+0747, with dispersion from intervening free electrons removed*




*Schematic diagram of a rotating radio pulsar shows its strong magnetic axis inclined to its spin axis. Pulsars have magnetic field strengths between 100 million and 1 trillion gauss. The fastest radio pulsar known spins 642 times per second.*

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### Leading-edge Methods in Atmospheric Imaging

B. Ellerbroek, C. Van Loan, N. Pitsianis, and R. Plemmons, "Multiple Control Bandwidth Computations in Adaptive Optics," *SIAM Journal on Optimization* (July 1996).

J. Nagy, T. Torgersen, and R. Plemmons, "Fast Restoration of Atmospherically Blurred Images," *Proceedings SPIE-94*, San Diego, Vol. 2296, pp. 542-553.

### Statistical Modeling of Radar Sea Clutter

D.W.J. Stein, "Detection of Random Signals in Gaussian Mixture Noise," *IEEE Transactions on Information Theory* **41**(6), Nov. 1995.

D.W.J. Stein, "Robust Detection of Random Signals in Exponential Noise," in *Proceedings of the IEEE Twenty-Ninth Asilomar Conference on Signals, Systems, and Computers*, Pacific Grove, California, 30 October – 1 November 1995.

# Forces Modeling and Simulation/C4I

*Forces Modeling and Simulation/Command, Control, Communications, Computers and Intelligence focuses on research that uses HPC for providing Dominant Battlespace Knowledge. Applications tend to be large, complex, and interactive. Progress in developing these types of systems continues with the development of architectures and components. The delivery of integrated systems remains as a future objective. This application area is receiving additional emphasis with the current initiation of CHSSI projects in FMS and the rapid advancement of information access through the World Wide Web technology. This year's success stories address the complexities of simulating military operations in an urban environment, Discrete Event Dynamic System (DEDS) modeling techniques, the development of a Master Environmental Library (MEL), and the use of massively parallel processors to simulate large numbers of synthetic forces.*

Mr. Robert A. Wasilausky
Navy Command, Control and Ocean Surveillance Center (NRaD)
San Diego, CA
CTA Leader for FMS

# Physics-based Dynamic Urban Combat Environments

V.A. To, T.A. Purnell, M.A. Thomas, R.J. Pearson,
W.Q. Zhou, A.M. Neiderer, and G.L. Brooks
*Army Research Laboratory, Aberdeen Proving Ground, MD*

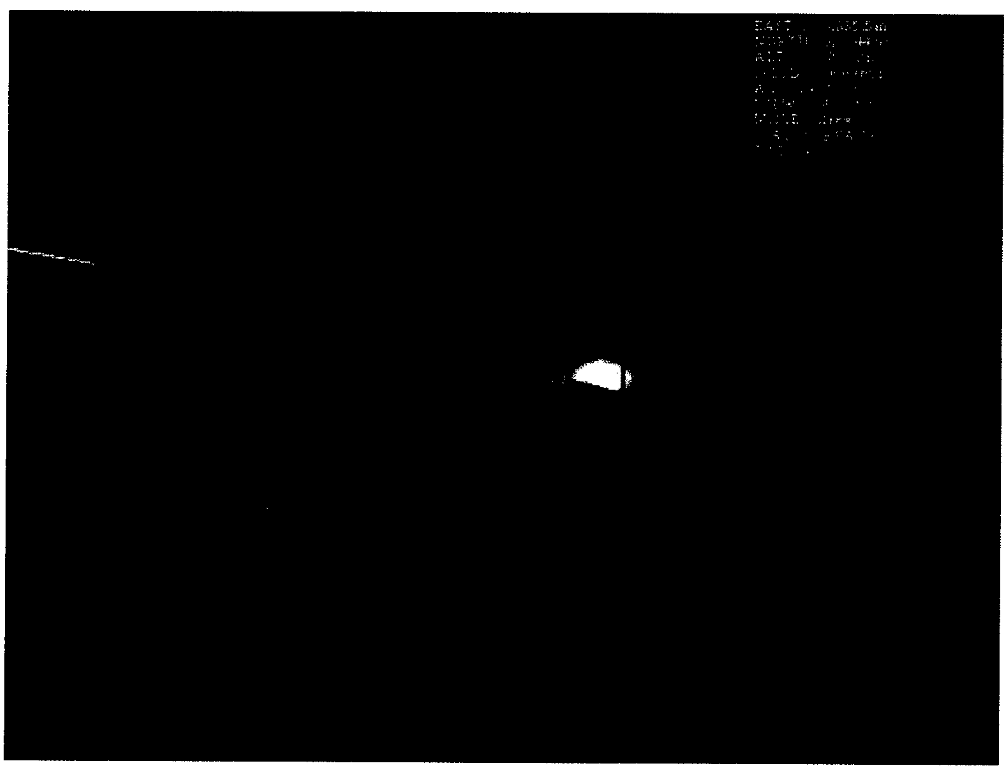
***Computer Resource:*** SGI Power Challenge Array [ARL MSRC]

***Research Objective:*** To implement high-fidelity physical models in real-time interactive combat simulations using HPC resources.

***Methodology:*** Many existing simulations of military operations in urban terrain (MOUT) use combat environments that are static in nature and not based on real physical data. The Army Research Laboratory (ARL) is conducting research toward developing interactive MOUT simulations that are both highly dynamic and physically realistic. The approach is to implement physics-based models in real time or near-real time. This is accomplished by using high performance computing platforms under a distributed computational environment.

***Results:*** A prototype distributed computing architecture (DCA) for interactive simulation has been developed at ARL. Several physics-based models were implemented under this DCA that incorporate the SGI Power Challenge Array located at Aberdeen Proving Ground, MD. These models include a detailed smoke model, a dynamic cratering model, and a model of weapons effects on urban structures. These models were successfully executed in real time using the SGI Power Challenge Array and provide realistic data to an ARL interactive MOUT simulation test-bed.

***Significance:*** Physically based simulations provide significantly more realism, which offers firefighters, soldiers, and law enforcement officers the capability to train and rehearse in a safe, controlled environment. Computer simulations can be used to create more hazardous environments than could be safely possible with mock ups. More realistic training time helps trainees to react more quickly and appropriately in life-threatening situations.



*Dynamic urban environment*

# DEDS Modeling Techniques and Voice/Data Integration

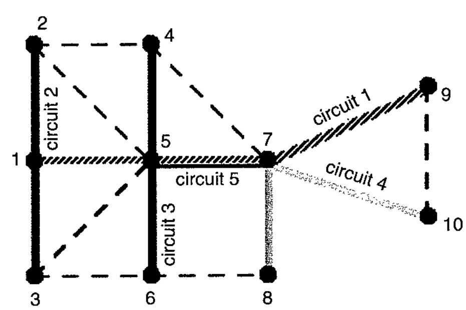
J.E. Wieselthier and C.M. Barnhart
*Naval Research Laboratory, Washington, DC*

***Computer Resource:*** TMC CM-5E [NRL DC]

***Research Objective:*** To develop modeling, evaluation, and control techniques for Discrete Event Dynamic Systems (DEDS). Specifically, we investigated the development of analytical and simulation techniques for the determination of good voice-call admission-control policies in integrated voice/data communication networks, for which practical exact analytical network models are not generally available.

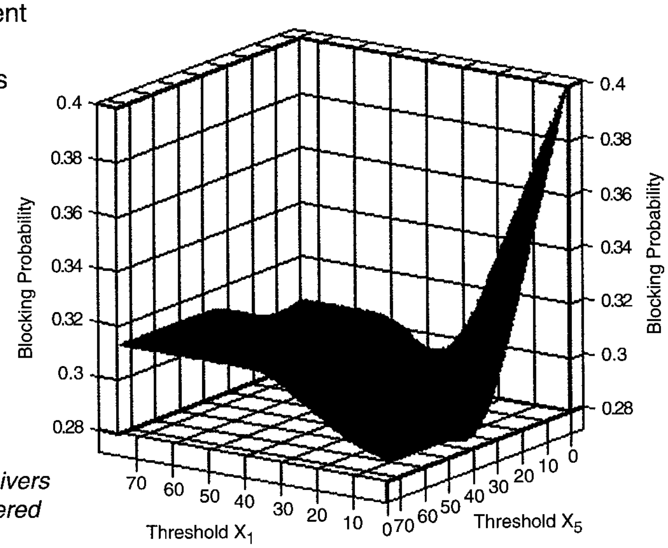
***Methodology:*** We developed "Standard Clock" (SC) parallel simulation models for integrated networks, with the goal of determining the optimal policy. The SC approach "parallelizes" simulation by passing a common event stream to a large number of problem instances, each of which updates its state subject to its unique admission-control policy. In conjunction with the SC framework, we have used "ordinal optimization" techniques that permit the rapid determination of good control policies after short simulation runs, thereby significantly reducing simulation time.

***Results:*** We have demonstrated the effectiveness of SC and ordinal optimization techniques for the rapid determination of good control policies for wireless integrated voice/data networks. Our studies have shown that the SC simulation technique has excellent scalability properties on the CM-5E, thus enabling the study of considerably larger problems than can be handled by sequential machines. For problems as large as 16,384 instances, SC simulation time appears to be virtually independent of problem size. The figure shows performance results for a wireless network that supports multihop circuit-switched connections between five source-destination pairs. A new call is admitted as long as a transceiver is available at every node along the path, and as long as the admission-control threshold associated with that call type is not exceeded. In this example, we want to find the thresholds for circuits 1 and 5 that minimize the overall blocking probability, for the case in which the thresholds on the other call types have been specified. Performance results were generated simultaneously for 5776 admission-control policies, permitting the selection of the policy that provides the best performance.




Example Network

***Significance:*** Techniques developed in this study can serve as the basis for the efficient operation of integrated voice/data communication systems, as well as other examples of DEDS such as manufacturing systems. These techniques are especially well suited for the parallel computing environment of the CM-5E. Our results suggest that short simulation runs and simple performance models are adequate for determining good control policies (even though they may not predict actual performance accurately). Thus, these techniques are practical for military and other applications in which high-performance computers are not available.




*Blocking probability vs thresholds $X_1$ and $X_5$ on circuits 1 and 5 in the example network (100 transceivers per node; thresholds = 75 on circuits 2, 3, and 4; offered load to each of the five circuits = 56.25 Erlangs)*

# Master Environmental Library

R. Allard
*Naval Research Laboratory, Stennis Space center, MS*
D.S. Ko
*Sverdrup Technology Inc., Stennis Space Center, MS*

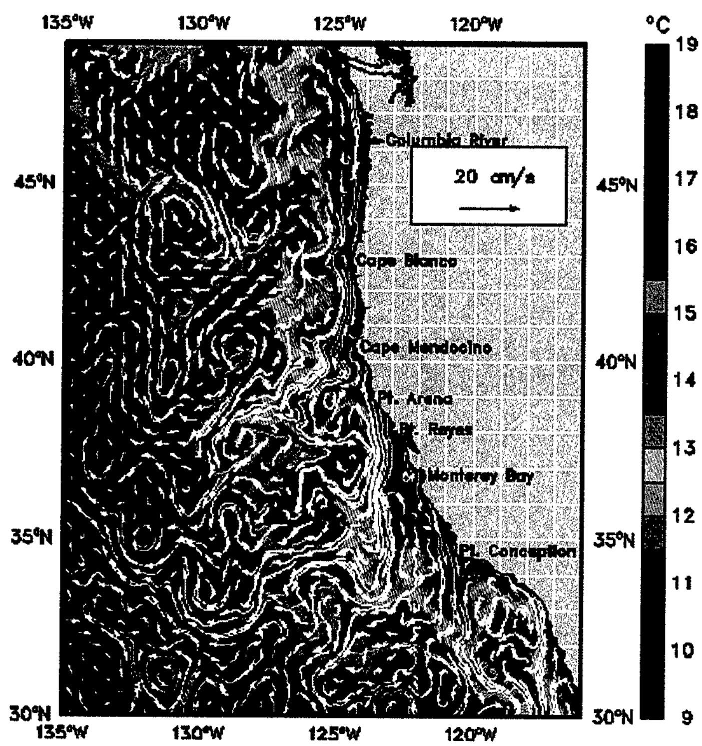
***Computer Resource:*** Cray C916 [CEWES MSRC and NAVOCEANO MSRC]

***Research Objective:*** To develop, demonstrate, verify, and validate a four-dimensional digital prototype DoD master environmental library (MEL). Standard atmospheric, oceanographic, or near-space databases do not exist today that provide a detailed, consistent, natural environment in a common format and in an accessible library.

***Methodology:*** To test the prototype MEL architecture, an integrated synthetic scenario is being developed for the southwest United States for a winter and summer period. Atmospheric and oceanographic models are being identified to be run for the littoral zone near Camp Pendleton, California. One such oceanographic model under development at the Naval Research Laboratory (NRL) is the Princeton West Coast (PWC) ocean model. The PWC model is an adaptation of a sigma coordinate ocean model on a 1/12-degree spherical grid extending from the coast to 135°W, and from 30 to 49°N. The model contains 30 sigma levels in the vertical, with resolution concentrated near the top and bottom of the water column to resolve surface and bottom boundary layers near shore. The PWC model includes fresh water runoff from seven major rivers. Open boundary information from the Navy's 0.25-degree Global Layered Ocean Model is provided on the northern, southern, and western boundaries of the model domain.

***Results:*** The PWC ocean model has been tested with a series of long-term spin-up runs made from climatological initial conditions, climatological atmospheric forcing, and time-varying lateral boundary conditions. The model-predicted fields are reasonable and reflect the presence of a vigorously meandering California Current system with its associated eddies. Animations of model output show that PWC exhibits the characteristics of much of the oceanographic variability known to exist off the U.S. west coast.

***Significance:*** The high-resolution (~10 km) PWC ocean model is being developed and tested for operational use for the Navy. A notable attribute of the PWC model is its nesting with a marginally eddy-resolving global ocean circulation model, which provides its open boundary conditions. With the Navy's interest in the littoral zone, this model is capable of providing the navigator, war-fighter, and simulator access to an accurate 3-D representation of the coastal ocean environment.




*PWC model result for day 600, corresponding to August 31 of the second year of model simulation. The model is forced with climatological winds and is coupled to NRL's 1/4-degree, 5-layer global model. Equatorward-flowing alongshore winds produce upwelling of colder water along the coast.*

# Advanced Distributed Simulation

L.C. Schuette
*Naval Research Laboratory, Washington, DC*
J.M. Opper, W.P. Niedringhaus, and B.R. Winner
*Mitre Corporation, McLean, VA*

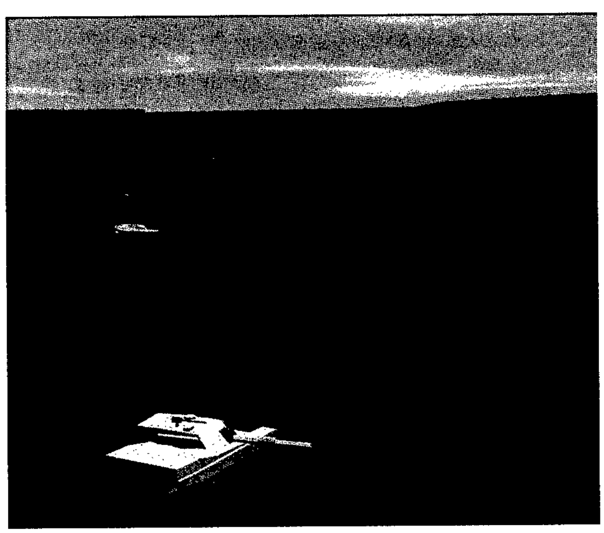
***Computer Resources:*** Cray T3D [AFDTC DC]

***Research Objective:*** To investigate strategies for using massively parallel processors to simulate large numbers of synthetic forces by using a contemporary synthetic forces software system.

***Methodology:*** Alternative functional decompositions of the software were developed that map to specific parallel programming paradigms. Factors are identified that constrain candidate implementation paths. Partitioning and filtering techniques are considered that can be used to reduce or eliminate broadcast packet distribution in a message-passing system. Data distribution, partitioning, and locking techniques are presented to support use of private, near-shared, and globally shared memory on a true shared-memory system.

***Results:*** In addition to examining partitioning schemes to provide an initial indication of the performance of the message-passing implementation, we devised a simple test program that exercised the core simulation services. This program created notional (or behaviorless) entities that performed a random walk over the terrain and generated entity state packet datagram units (ESPDUs) at specified intervals. Static terrain partitioning was applied so that each ModSAF (a commonly used computer-generated forces simulation) processing element (PE) simulated entities over a specified terrain area. The terrain was allocated to the PEs based on a simple row/column assignment mechanism. The first series of tests performed broadcast distribution of all generated ESPDUs for varying numbers of processing elements. The data gathered during these tests included the packet send and receive rates, the number of locally simulated (owned) entities, the number of perceived but not simulated (reflected) entities, the total number of entities simulated, and the performance of the ModSAF event scheduler. We then repeated the test series with relevance filtering activated. In this series, each entity expressed interest in receiving state data for all other entities residing in cells within a specified radius. All ESPDUs were multicast to all PEs having expressed interest in the originating cell.

***Significance:*** Simulation is becoming an increasingly important component of the DoD technology base. In particular, Distributed Interactive Simulation (DIS) is being used more frequently to support simulated environments for training and concept evaluation. Although DIS has demonstrated its utility in small-scale applications, potential uses require scaling the technology to support substantially larger scenarios involving 10,000 to 100,000 entities.



*Simulated battlefield*

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# Environmental Quality Modeling and Simulation

*The Department of Defense has more than 10,000 contaminated sites on its active installations within the United States that may require some level of subsurface environmental restoration. DoD also has significant natural and cultural resources stewardship responsibilities (e.g., habitat management for threatened and endangered species). Failure to properly steward these resources has been shown to directly affect training and, hence, readiness and environmental security. The Environmental Quality Modeling and Simulation (EQM) computational technology area is providing DoD with state-of-the-art modeling systems in support of environmental risk management, optimal site cleanup, and environmentally sustainable training activities.*

*The EQM success stories presented herein represent the range of scales associated with the research and development challenges DoD faces in meeting its EQM requirements. Two of the stories report basic science investigations of subsurface pore-scale flow and transport mechanics where the fundamental spatial scale is microns to millimeters. Two related stories describe the development of network modeling approaches that may provide the key to scaling pore-scale dynamics up to engineering-scale (e.g., meters) calculations, and the interactive visualization required to empower rigorous evaluation of the results of network and pore-scale modeling investigations. Two additional stories report ongoing investigations of improved engineering-scale subsurface flow, contaminant transport, and remediation-alternative modeling and simulation methods, with emphasis on scalability and adaptive grid refinement.*

*A representative discussion of success in EQM research and development would, of course, be incomplete without examples of the incompressible Navier-Stokes solvers being developed for optimal and environmentally sustainable design and operation of strategic waterways (e.g., home ports, harbors, and/or major navigable rivers). These two specific examples illustrate the coupling of three-dimensional incompressible Navier-Stokes solution techniques with the integration of transport equations for multiple constituents (illustrated here for salinity), and the development of computationally efficient adaptive free-surface solution techniques.*

Dr. Jeffery P. Holland
Army Engineer Waterways Experiment Station
Vicksburg, MS
CTA Leader for EQM

# Fingered Flow Modeling

J.L. Nieber, D. Misra, and H.V. Nguyen
*ARL/Army High Performance Computing Research Center, Minneapolis, MN*

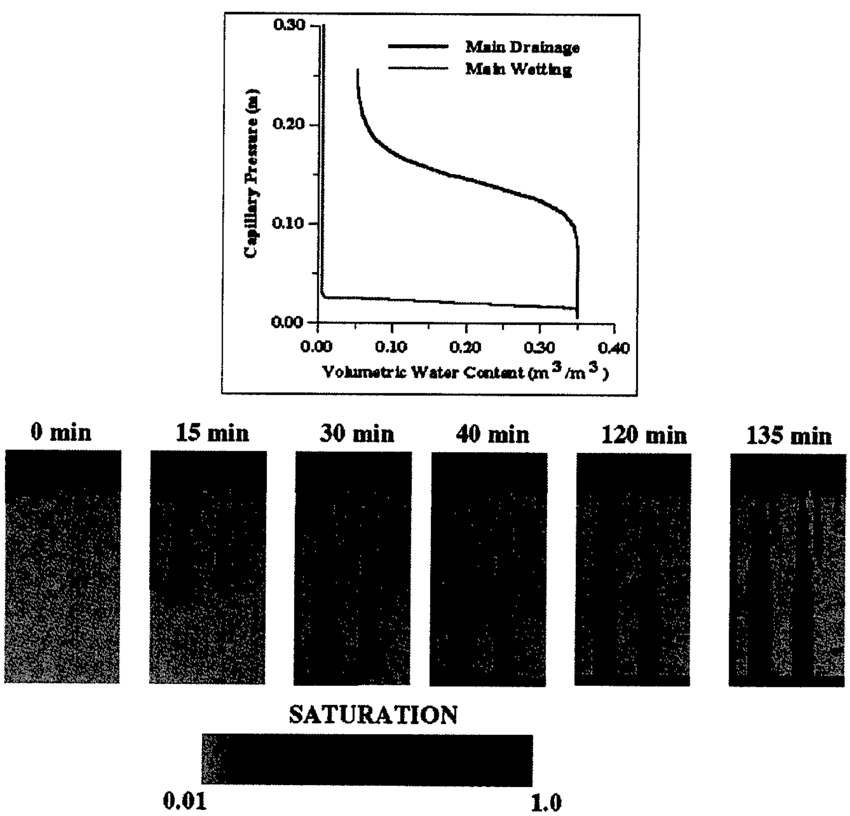
***Computer Resource:*** Cray C916 and Cray X-MP [AHPCRC DC]

***Research Objective:*** To develop a two-dimensional model for simulating gravity-driven unstable (fingered) flow in unsaturated porous media such as soil. This requires understanding the physics of flow in unsaturated porous media, the process of hysteresis that the flow undergoes during drainage and imbibition, and the subtle initiation of the instability of the flow in the model. This model can be used to study preferential flow and transport of contaminants from chemical spills and spills of nonaqueous liquids.

***Methodology:*** The two-dimensional form of the Richards equation is solved for a multiphase flow environment by using a Galerkin finite-element method with a Picard iteration scheme, adaptive time stepping, and preconditioned conjugate gradients. The initiation of the finger is accomplished by using an initial random perturbation in the field of flow.

***Results:*** The results obtained have shown qualitative comparison with laboratory-scale experimental results. This effort is the first successful attempt at mathematically modeling the gravity-driven fingered flow process.

***Significance:*** Chemical spills are becoming an increasing problem today. These chemicals can move rapidly to ground water through preferential flow paths such as gravity-driven unstable flow. We need to better understand this unstable flow process and the associated preferential transport of chemicals so that prevention and clean up methods can be improved.




*Saturation profiles during a wetting/drainage/re-wetting application, illustrating the formation and persistence of fingered flow in an unsaturated porous media. The inset shows the soil moisture characteristic function used for the modeling. (First wetting occurs for 0-30 minutes, drainage from 30-120 minutes, re-wetting 120-150 minutes.)*

# Free-Surface Flows Over Hydraulic Structures

M. Behr and T. Tezduyar
*ARL/Army High Performance Computing Research Center, Minneapolis, MN*
R. Stockstill and R.C. Berger
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

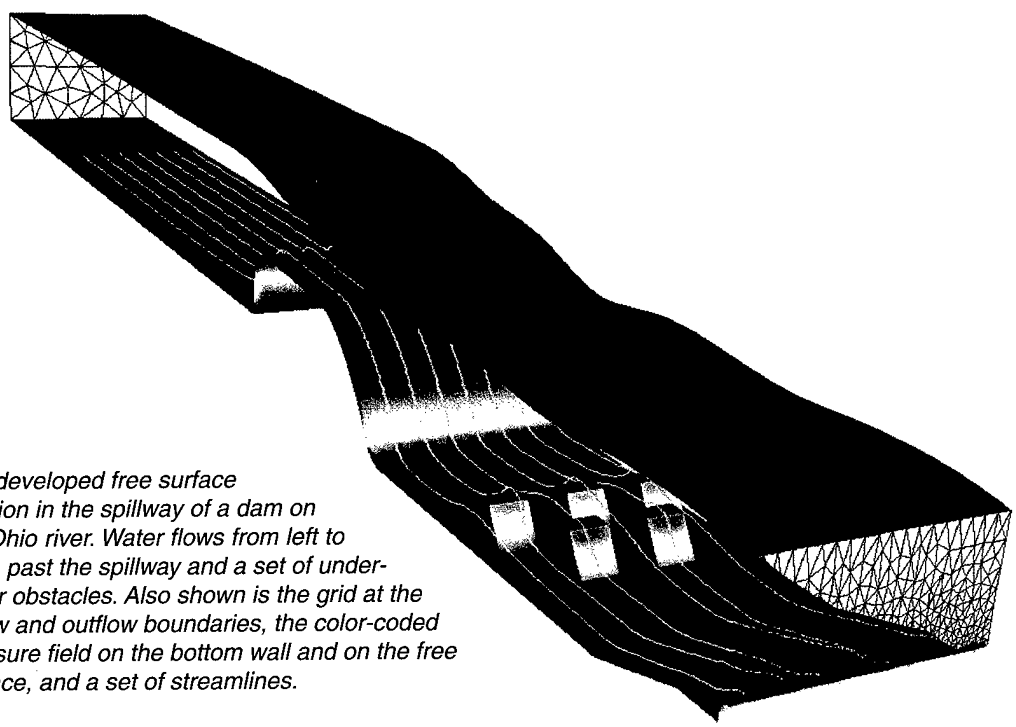
***Computer Resource:*** TMC CM-5 [AHPCRC DC]

***Research Objective:*** To develop tools for the design and evaluation of hydraulic structures such as dams and channels, and for analyzing hydraulic conditions in strategic waterways. The developed techniques must be applicable to the complicated geometries of structures and must take advantage of the increased resolution offered by scalable parallel implementations.

***Methodology:*** Three-dimensional Navier-Stokes equations for incompressible flow are discretized by using a stabilized space-time finite-element formulation for deforming spatial domains; the resulting coupled equations are solved by using an iterative solution technique. The unstructured tetrahedral mesh is moved according to the displacement of the free surface by using the finite-element formulation of linear elasticity equations.

***Results:*** Highly turbulent flows for a structure on a major strategic waterway (the Ohio river) were computed and compared with experimental results obtained from the Army Engineer Waterways Experiment Station. Evolution of the free surface and velocity and pressure fields were obtained and visualized.

***Significance:*** The new capability of rigorous simulation of free-surface problems on scalable architectures reduces the need for physical experimental investigation of multiple scenarios, thereby reducing costs and turnaround time for waterway evaluation and design optimization.



*The developed free surface position in the spillway of a dam on the Ohio river. Water flows from left to right, past the spillway and a set of underwater obstacles. Also shown is the grid at the inflow and outflow boundaries, the color-coded pressure field on the bottom wall and on the free surface, and a set of streamlines.*

# Pore-Scale Flow and Reactive Transport

H.T. Davis, Y.E. Kutsovsky, and R.S. Maier
*ARL/Army High Performance Computing Research Center, Minneapolis, MN*
R.S. Bernard and S.E. Howington
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

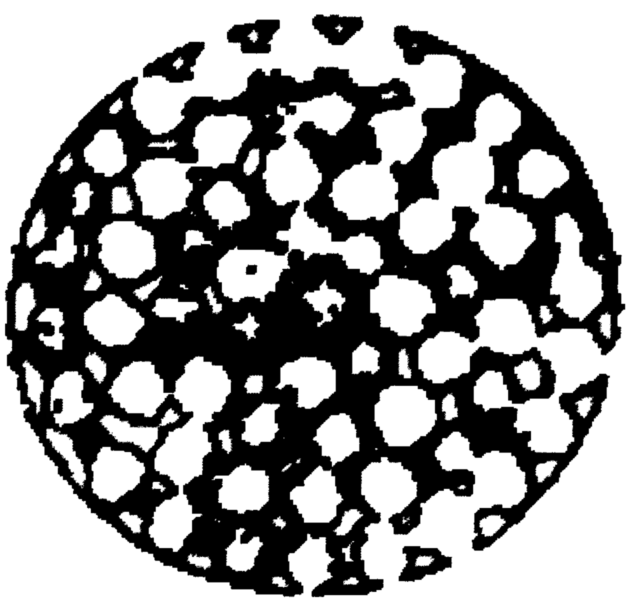
***Computer Resource:*** Cray C916 and TMC CM-5 [AHPCRC DC]

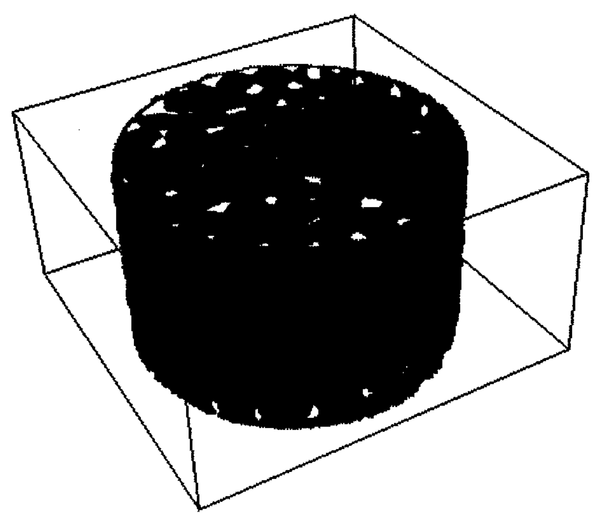
***Research Objective:*** To establish reliable computational methods for developing mass transfer coefficients and correlations needed to calibrate field-scale simulations of contaminant transport.

***Methodology:*** The lattice Boltzmann (LB) method is useful in simulating complex hydrodynamic flows at low Reynolds numbers. The method recovers Navier-Stokes dynamics using a formulation based on kinetic theory. A related formulation recovers dynamics of the advection-diffusion equation, and is used to model reactive species transport in a bulk liquid. Data-parallel codes for three-dimensional LB hydrodynamics have been developed and evaluated on the Cray C916, T3D, the CM-5, and workstation arrays.

***Results:*** Three major conclusions about the suitability of this approach for high performance computing have been drawn. LB methods are scalable, LB models tend to be memory-limited (not CPU-limited), and high performance Fortran or Fortran 90 is a very desirable programming model for LB methods. Additionally, numerical investigations have identified the errors associated with hydrodynamic calculations at various scales and provide a basis for determining the reliability of the calculations.

***Significance:*** LB methods and available massively parallel computers allow for detailed calculation of the interfacial area between separate liquid and solid phases. These calculations are crucial to development of mass transfer correlations. Such correlations are key components of reliable subsurface models required for military installation cleanup.





*Cross section (left) and perspective (right) of simulated axial fluid velocity in a cylinder packed with glass beads*

# Shared Exploration of Immiscible Contaminant Flow

J.E. West, A.R. Carrillo, S.E. Howington, and D.A. Horner
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

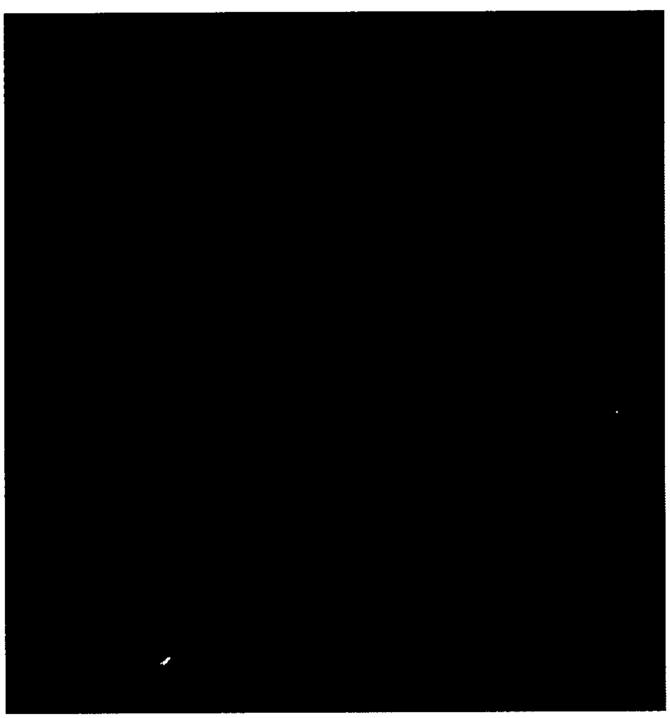
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To develop an interactive visualization system operating on a range of high performance computing (HPC) architectures in support of both collaborative and independent exploration of large volumetric, geohydrologic data sets.

***Methodology:*** The core of this visualization system is a highly optimized volume-rendering engine designed to operate in the type of HPC environments in which numerical simulations are performed. Users interact with the visualization through a client running on a local workstation that mediates all user interaction. The client supplies updated viewing information to the volume renderer as the user manipulates the view, and also displays the newly created images to the user as they arrive. The system further extends the remote visualization mechanism by providing support for collaborative exploration of the data by multiple remote users, and by enabling visualization of time-varying data.

***Results:*** The visualization shown illustrates pore-scale displacement of a wetting fluid, such as water, by an immiscible liquid contaminant (for example, an organic solvent) in a porous medium. Such investigations provide insight into pore-scale processes and someday may augment expensive and time-consuming laboratory tests. The image shown was rendered at more than 18 frames per second, with multiple light sources from a data set containing more than eight million entries.

***Significance:*** Leveraging HPC resources in volume visualization allows researchers to explore data without experiencing the delays caused by performance and memory factors typically encountered on workstations. Optimal performance is crucial in that the ability to interact in real time with a volume visualization has been identified as central to a thorough understanding of the three-dimensional and time-varying relationships inherent in volume data.



*Displacement of wetting fluid by an immiscible liquid contaminant in a porous medium*

# Cleanup Strategies Within DoD

J.P. Holland and M.S. Dortch
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

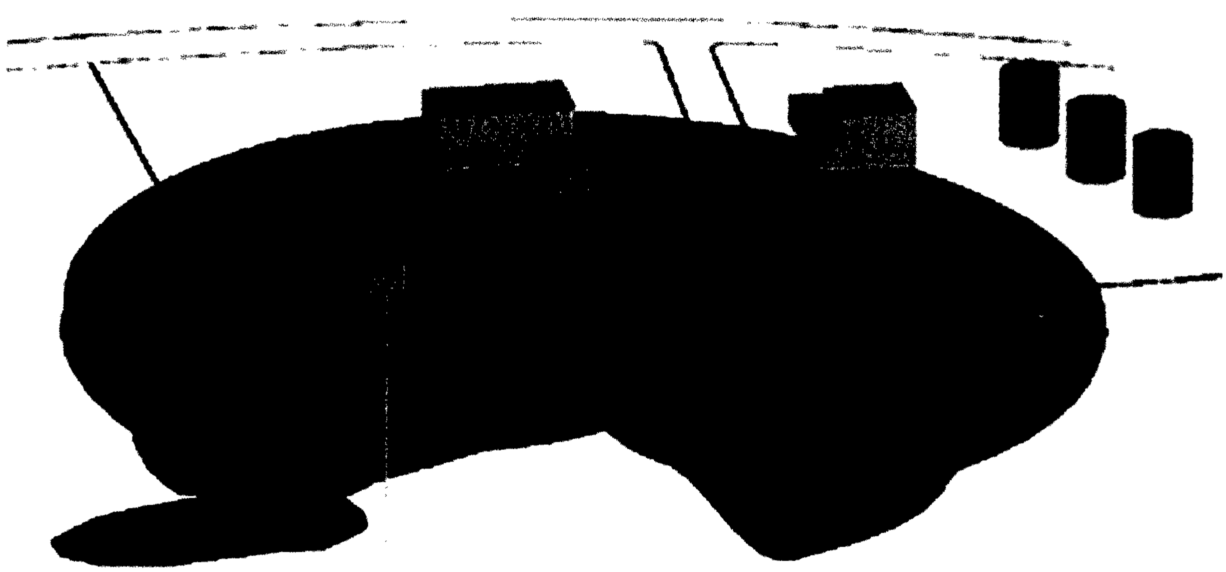
***Computer Resources:*** Cray C916 and Y-MP [CEWES MSRC]

***Research Objective:*** To couple state-of-the-art three-dimensional subsurface flow and transport models with 15 to 20 remediation alternative simulators for evaluating and optimizing clean-up scenarios prior to their implementation at military sites.

***Methodology:*** Three-dimensional (3-D), time-varying subsurface flow and contaminant transport models, involving finite-element and finite-volume solutions of the modified Richards equation (for flow) and the advection-diffusion equation (for transport with up to 20 state variables), are being computationally coupled to remediation simulation routines. The calculations involve solution of millions of equations routinely. Two-dimensional hydrologic simulations of precipitation, surface runoff, and infiltration are being coupled to the 3-D simulators to allow accurate hydrologic forcings on military clean-up activities. These calculations presently tax the largest HPC resources within DoD.

***Results:*** Significant savings in the proposed costs of remediation alternatives at DoD sites have already been achieved through the use of these modeling tools.

***Significance:*** DoD has more than 10,000 installation sites that may require some level of cleanup. Estimates of clean-up costs for these sites, 85% of which have experienced contaminated groundwater resources, are more than $45 billion. Numerical simulation of cleanup alternatives are expected to save a minimum of 5-10% of the costs of these cleanups.



*Desktop visualization of the DoD Groundwater Modeling System, showing a conceptualized contaminant plume (surface features and one observation well superimposed)*

# Hydrodynamic, Salinity, and Shoaling Investigation for Strategic Waterway Modifications

R.T. McAdory, Jr. and C.J. Callegan
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

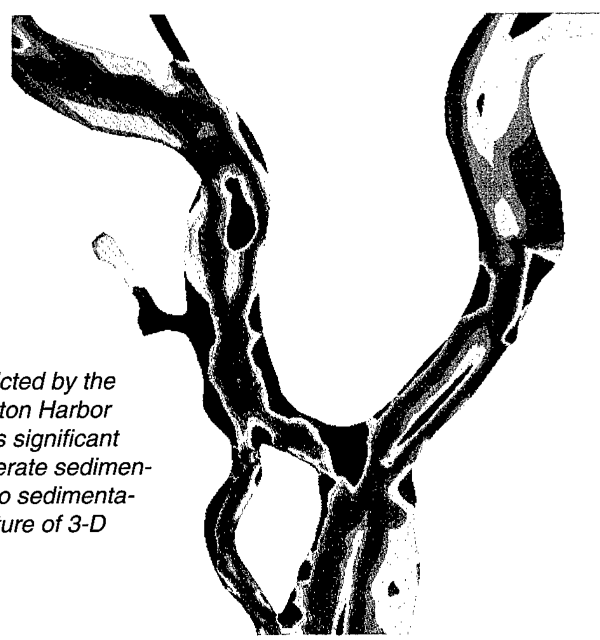
***Computer Resource:*** Cray C916 and Y-MP [CEWES MSRC]

***Research Objective:*** To investigate the potential hydrodynamics, salinity, and shoaling impacts associated with operational modifications to a strategic national port—the Charleston Harbor, S.C. Expansion Project.

***Methodology:*** Three-dimensional (3-D) calculations for hydrodynamics, salinity, and sedimentation are being computed for the Charleston Harbor. These simulations use the RMA suite of models maintained by the Army Engineer Waterways Experiment Station. Experiments were conducted using existing and three planned channel configurations. The 3-D model allowed density and other 3-D effects to be fully accounted for in the complex harbor.

***Results:*** Significant improvement has been achieved in optimizing salinity and sedimentation levels as a function of the proposed waterway geometry. These calculations have proven to be a direct basis for comparison of different waterway plans and their environmental and navigation efficiencies by federal, state, and local agencies.

***Significance:*** This nation has thousands of miles of harbors and waterways whose navigation is essential to move troops and material during combat. Environmentally and economically sustainable engineering management of these waterways is essential to their continued effectiveness. This is particularly true of sedimentation in the waterways because of resulting navigation difficulties and dredging costs due to shoaling. The dual-use modeling technology employed in this study is a key technology used by resource agencies to determine the environmental "fitness" of waterway design. Confidence in these calculations is a key to their acceptance by regulators and other decision makers.



*Significant sediment accumulation is predicted by the model in strategic locations of the Charleston Harbor and its associated channels. Red indicates significant shoaling, yellow and orange indicate moderate sedimentation, and green to blue indicate little to no sedimentation. RMA10-WES provides a detailed picture of 3-D hydrodynamics in these zones.*

# Hydrologic Modeling for Environmental Quality Analysis of Military Installations

J.H. Schmidt
*Army Engineer Waterways Experiment Station, Vicksburg, MS*

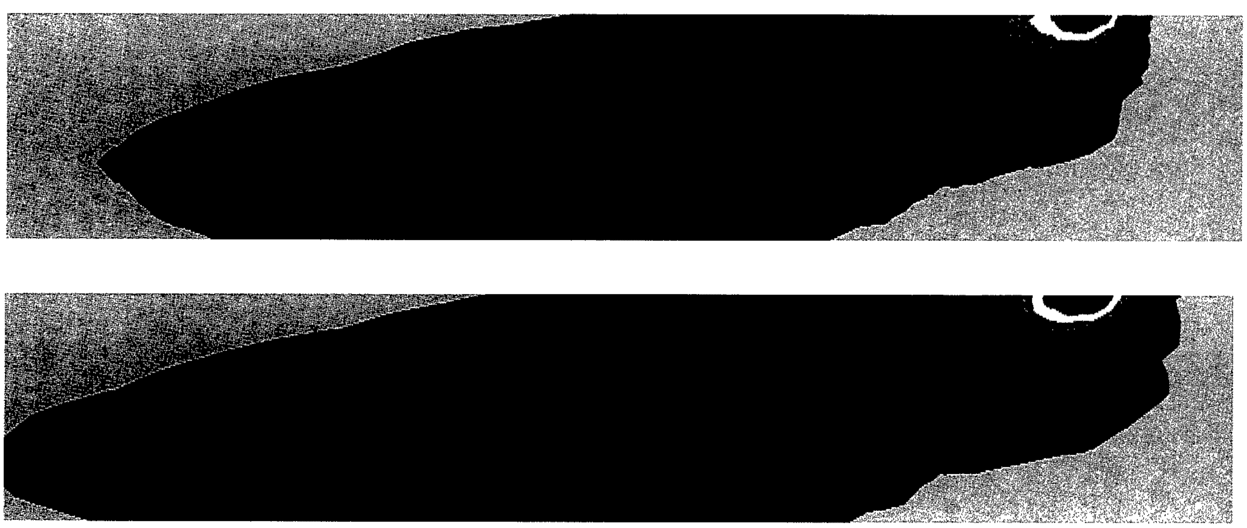
***Computer Resource:*** Cray C916 and Y-MP [CEWES MSRC]

***Research Objective:*** To develop a more accurate and efficient hydrologic model of contamination and remediation processes for applications at military installations.

***Methodology:*** Current production codes for hydrologic problems are not as efficient or as robust as many of the "research" codes used by individual researchers. The ADaptive Hydrology (ADH) model incorporates many state-of-the-art numerical techniques in a model of hydrologic processes. Model features include: unstructured grids for tortuous geologic features; adaptive gridding for moving fronts and boundary layers; modern stabilization schemes for convection-dominated problems; and error indicators for quality control. The ADH model also solves physical problems such as two-phase flow (which gives it the capability to model remediation techniques such as air sparging) that are not typically found in current production codes.

***Results:*** Tools previously available only to hydrologic researchers are now available to DoD engineers to analyze and develop hydrologic resources. Modeling capabilities have been significantly improved in terms of accuracy, efficiency, and physical processes.

***Significance:*** The DoD has a responsibility to develop and maintain the ecosystems of its many installations. A significant part of these systems is the hydrologic environment. This work gives DoD engineers improved tools to assess the hydrologic environment and make sound management decisions.



*Both images show a plume developed from a spill site under identical circumstances. The upper image uses adaptive refinement, the lower image does not. Note that the better resolved plume is significantly shorter, emphasizing the important role of adaptive refinement for groundwater management.*

# Discrete Network Modeling of Flow and Transport Through Porous Media

J.F. Peters and S.E. Howington
*Army Engineer Waterways Experiment Station, Vicksburg, MS*
R.S. Maier
*ARL/Army High Performance Computing Research Center, Minneapolis, MN*

***Computer Resource:*** Cray T3D [AHPCRC MSRC]

***Research Objective:*** To develop discrete models based on fundamental physics to capture complex processes in flow and transport through porous media.

***Research Methodology:*** Particulate materials defy realistic analysis by conventional continuum mechanics on which traditional numerical models are based. As an alternative, models based on mechanics of discrete media have been created. Model practicality comes from the ability to "coarsen" the system to reduce the number of degrees of freedom to that feasible for available computing resources. The number of degrees of freedom required for accurate modeling depends on the smallest scale to be modeled accurately.

***Results:*** The network depicted in the graphic contains about 21,000 connections and 50,000 paths. The concentration field shows the network capturing correct behavior near a continuous source and in the plume downstream. A continuum model, based on the advection-dispersion equation with macroscopic coefficients, will incorrectly predict significant upstream spreading. This network model represents minimal problem size for practical applications.

***Significance:*** Application of the model to assess cleanup technologies requires three-dimensional representation of the medium under transient multiphase flow conditions with addition of diffusive, chemical, thermal, and electrical processes. High performance computing provides the means to bridge the gap between theoretical development and practical application.

*The discrete network (top) represents the porous medium. When spatially averaged, the resulting concentration field (bottom) reflects accurate representation of dispersion physics.*

# Selected References


### Fingered Flow Modeling

J.L. Nieber, "Modeling Finger Development and Persistence in Initially Dry Porous Media," *Geoderma* **70** (1996).

### Free-Surface Flows Over Hydraulic Structures

M. Behr and T.E. Tezduyar, "Finite Element Solution Strategies for Large-Scale Flow Simulations," *Computer Methods in Applied Mechanics and Engineering* **112**, 3-24 (1994).

### Pore-Scale Flow and Reactive Transport

Y.E. Kutsovsky, L.E. Scriven, H.T. Davis, and B.E. Hammer, "NMR Imaging of Velocity Profiles and Velocity Distributions in Bead Packs," *Physics of Fluids A* **8**(4), 1-9 (1996).

R.S. Maier, Y.E. Kutsovsky, S. Nivarthi, H.T. Davis, D.W. Grunau, S. Howington, and R.S. Bernard, "Pore-Scale Flow and Transport Calculations Using the Lattice Boltzmann Method," in *Proceedings of the Conference on Next-Generation Environmental Models*, edited by M. Wheeler and G. Delic, Bay City, MI, August 1995 (SIAM, 1996).

*Advanced computational methods are being used to model and simulate complex electronics to explore new concepts, gain insight and improved understanding of the underlying physics, and perform virtual prototyping and test new ideas. Given the importance of state-of-the-art electronics as an enabling technology in most DoD systems, the impact of high-performance computing to the development, design, analysis, and proof of concept of innovative electronics technology is substantial.*

*The Computational Electronics and Nanoelectronics effort is very diverse; it covers a variety of device/circuit types and exploits a variety of numerical and predictive modeling and simulation techniques. The scope of this effort involves quantum electrophysics and energy transport, microstructural analysis, electromagnetics, network theory, and coupled nonlinear systems.*

*The following examples span a broad spectrum of mission requirements that demonstrate the pervasiveness and significance of electronics in DoD systems. The first two improve our understanding of the atomic details and novel properties of various electronic materials for improved computing and sensing. The next three deal with structural analysis of various microelectromechanical devices for device optimization and reduced acceleration sensitivity. The next two deal with electromagnetic analysis of high-frequency packages and interconnects for reduced parasitics. The final story involves nonlinear stochastic analysis of a large coupled array for ultra-sensitive magnetic sensing.*

# Computational Electronics and Nanoelectronics

Dr. Barry S. Perlman
Army Research Laboratory
Fort Monmouth, NJ
CTA Leader for CEN

# Travels with Silicon

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*North Carolina State University, Raleigh, NC*
*Office of Naval Research, Arlington, VA*

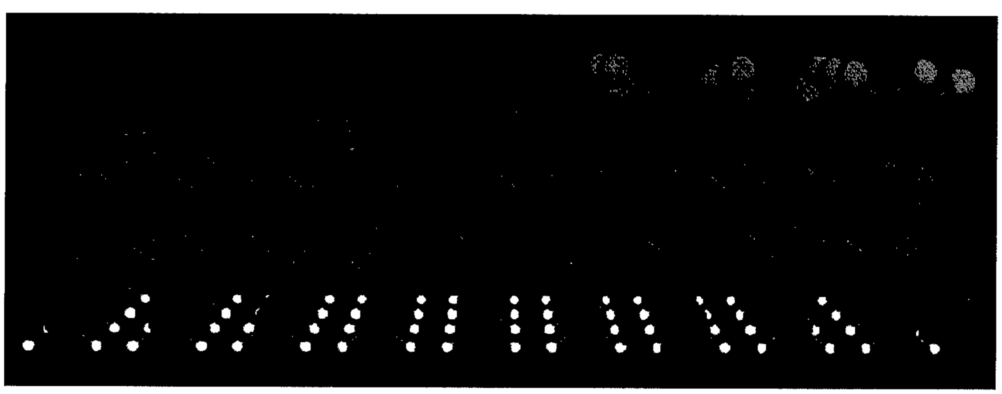
***Computer Resource:*** Cray T3D and Cray C90 at Pittsburgh Supercomputing Center

***Research Objective:*** To understand in atomic detail the growth modes of semiconductors and to identify the conditions for high-quality layer-by-layer growth. This project focuses on the "step-flow" mechanism, which is the most common growth process used in producing chip-quality crystals of silicon.

***Methodology:*** A powerful computational approach called quantum molecular dynamics (QMD) is used to simulate growth processes. This code is a truly quantum approach that allows the electrons and atoms to move freely with time, so that the atom-atom interactions are computed ab initio, directly from the electronic forces. The C90 adaptation of QMD runs at 693 Mflops on a single C90 processor, one of the fastest codes running on this machine. Taking advantage of Pittsburgh's new C90 in early 1993, a series of four-processor runs (2.3 Gflops) was carried out. These runs resulted in the first calculations to give the structure of steps. Further ab initio calculations on the C90 explored how adatoms move across the silicon surface, jumping from one inter-atomic space to the next, until they become incorporated in the step edges. To make this calculation feasible, these simulations were done at zero temperature and investigated only certain possible pathways. With the availability of the Cray T3D, it became feasible to do these calculations at high temperature, which more realistically simulates the silicon growth process as it occurs in reality. Using the T3D code, a series of heating up experiments have been conducted.

***Results:*** The results on the C90 showed the energy barriers that must be overcome for the adatom to "jump" and the binding sites where they end up. Results from the T3D heating experiments reproduced the high-temperature structure observed with scanning tunnelling microscopy, confirming the viability of the computational approach. Future simulations will probe for new and unforeseen diffusion mechanisms.

***Significance:*** For a range of commercial products, from VCRs to automobiles, as well as for the highest technology research and communications like the Space Shuttle and supercomputers, microelectronic "chips" are an indispensable foundation for 20th century living. Better understanding of the atomic details of silicon crystal growth will lead to better methods for producing defect-free crystals of silicon at low cost in commercial quantity, advancing computer chip technology.



*Three adatoms (red) are deposited on the surface of a seven-layer silicon slab, two on the lower terrace (violet), one on the upper (aqua). Silicon bulk atoms (blue) are sandwiched between the surface and a bottom layer (purple) saturated with hydrogen atoms (white)*

# Neither Antiferromagnet Nor Ordinary Metal: A Novel Metallic State

D.W. Hess
*Naval Research Laboratory, Washington, DC*
J.J. Deisz and J.W. Serene
*Georgetown University, Washington, DC*

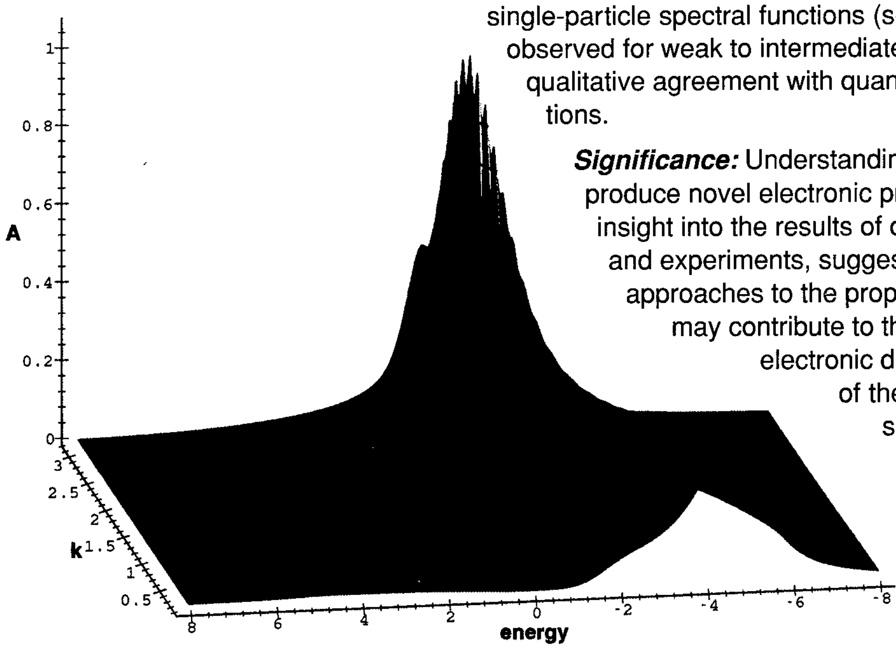
***Computer Resource:*** TMC CM-5E [NRL DC]

***Research Objective:*** To elucidate the role of antiferromagnetic spin-fluctuations in determining the nature of electronic excitations in materials such as the high-temperature superconductors. In these materials, electronic interactions, planar structure, and incipient magnetic order may act in concert to produce states that exhibit unusual long-range order, or unusual transport and thermodynamic properties. Antiferromagnetic spin-fluctuations may be responsible for unusual metallic properties and for an unusual, possibly "d-wave," superconducting state in yttrium barium copper oxide. A particular focus is the nature and evolution with decreasing temperature of electronic excitations (quasiparticles) at low energy. A further objective is to assess the accuracy of approximate theoretical methods that have been used to argue for the existence of d-wave superconductivity in the high-temperature superconductors.

***Methodology:*** The Hubbard Hamiltonian in two-dimensions, together with the fluctuation exchange approximation, is used as a self-consistent finite-temperature model for coupled quasiparticles and spin-fluctuations. A scalable parallel algorithm previously developed under the HPCMP for the TMC CM-5 enables accurate finite-temperature calculations of low-energy excitations and thermodynamic properties for this model.

***Results:*** With decreasing temperature, the coupling of quasiparticles to spin fluctuations results in the evolution of a metallic state unlike the Fermi-liquid state in an ordinary metal. This state exhibits no long-range magnetic order, but magnetic correlations are reflected in the nature of low-energy excitations and single-particle properties. For example, the density of states at the Fermi energy shows a dramatic reduction (a pseudogap), and "shadow structures" appear in single-particle spectral functions (see figure). These features, observed for weak to intermediate interaction strengths, are in qualitative agreement with quantum Monte Carlo calculations.

***Significance:*** Understanding how spin fluctuations can produce novel electronic properties provides physical insight into the results of other numerical calculations and experiments, suggests new computational approaches to the properties of these materials, and may contribute to the development of new electronic device technologies in support of the Navy's mission. The figure summarizes calculations that suggest an interpretation of structure observed in photoemission experiments on high-temperature superconductors and related materials.




*Momentum- and energy-dependent spectral function accessible to angle-resolved photoemission experiments. The prominent ridge on the right shows the dispersion of (single particle/hole) electronic excitations for momenta along the (100) direction in the half-filled Hubbard model at a temperature of ~100 K for an interaction strength of 1/2 the bare bandwidth. 'Shadow structure' appears as the smaller ridge to the left.*

# Finite-Element Modeling of Resonant Microelectromechanical Sensors

J.T. Stewart
*Army Research Laboratory, Fort Monmouth, NJ*

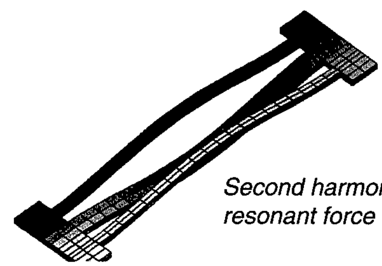
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To develop a general-purpose finite-element method for the direct numerical solution of small-amplitude vibrations of a crystal structure superposed on a (possibly finite) static biasing state. This is necessary to model the performance of resonant microelectromechanical (MEMS) sensors.

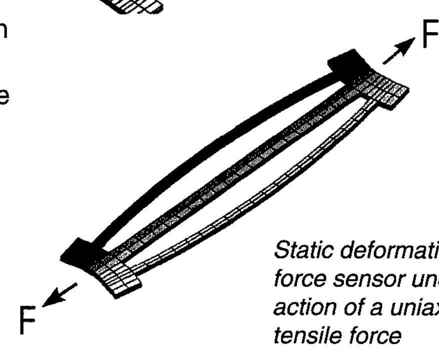
***Methodology:*** A general class of finite elements has been developed that is based on a general and rigorous theory for small fields superposed on a bias. The solution of the discretized problem is handled in two parts: (1) the solution of a static problem under the loading from the variable being sensed (e.g., acceleration, rate of rotation, pressure, force, strain); and (2) the construction and solution of a nonlinear vibration eigenvalue problem that incorporates the static solution vector into the effective spatially varying element stiffness properties via finite-element shape functions.

***Results:*** This code has been successfully used to model accelerometers, resonant strain gauges, and resonant force sensors fabricated from materials such as silicon, gallium arsenide, and quartz. The figure shows a study performed on an AT-cut quartz force sensor consisting of three beams that are piezoelectrically excited into flexural resonance under the biasing action of an axial force. These results show the generally different behavior that various harmonics may exhibit. Such information is crucial to the design of these structures.

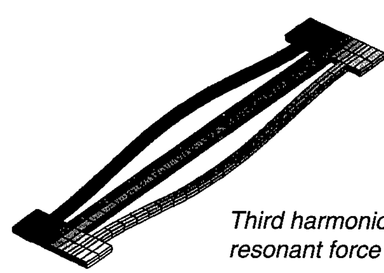
***Significance:*** The ability to simulate the performance of resonant MEMS devices allows the designer to explore different geometries and vibration modes for a particular application without making costly fabrication runs. The models developed with this code can be merged with circuit simulation to allow the designer to model the performance of the entire system.



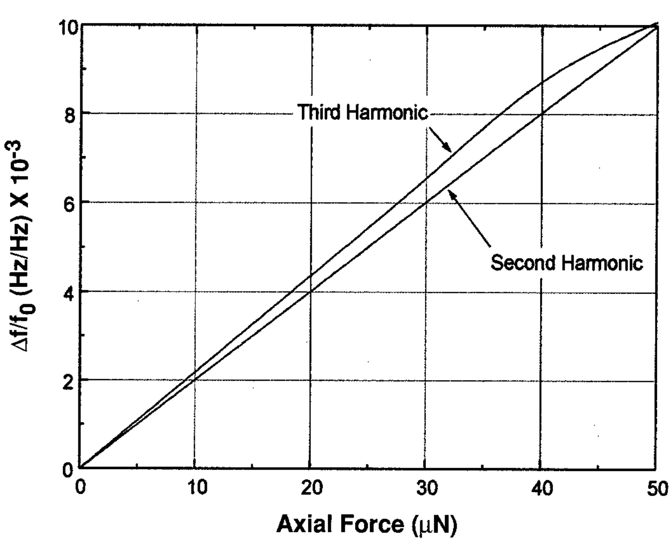
*Second harmonic for the resonant force sensor*




*Static deformation of the force sensor under the action of a uniaxial tensile force*



*Third harmonic for the resonant force sensor*




*Relative change in resonant frequency of second and third harmonics of the force sensor*

# Geometrically Nonlinear Finite-Element Modeling of Microelectromechanical Structures Subjected to Electrostatic Loading

J.T. Stewart
*Army Research Laboratory, Fort Monmouth, NJ*

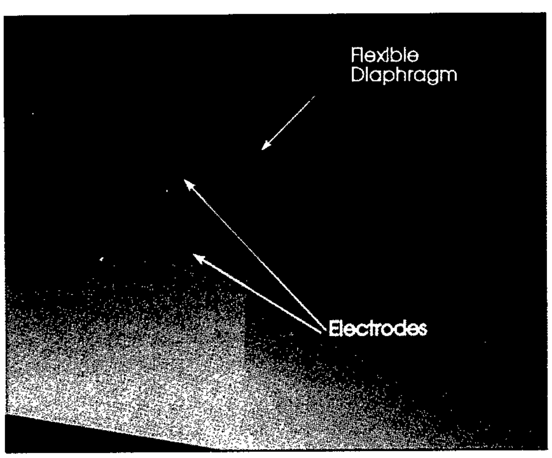
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To develop a general and consistent hybrid nonlinear finite-element/boundary-element method for modeling the deformations in an elastic structure under the action of electrostatic forces to aid in the design of microelectromechanical systems (MEMS) that use electrostatic actuation.

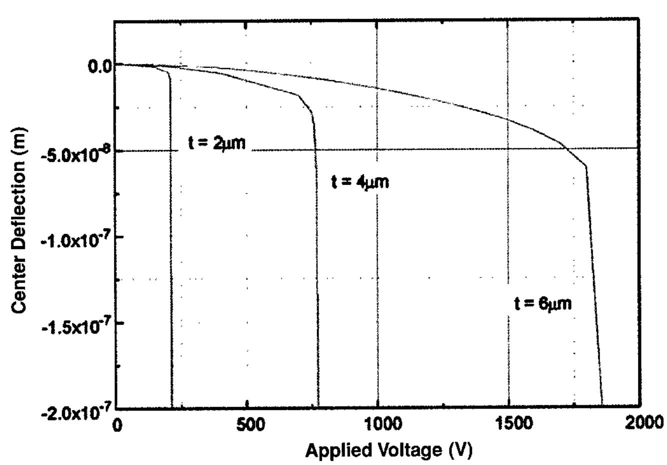
***Methodology:*** A general and rigorous incremental nonlinear finite-element method has been developed that uses a boundary-element solution at each load step to update the electrostatic force on the body. The incremental finite-element method is based on the assumption of small strains with large rotations and deformation-dependent loading conditions, giving rise to the so-called geometric nonlinearity. The same family of interpolation functions is used for the finite-element and boundary-element models, which facilitates a rigorously correct representation of the electrostatic force at each element integration point from the boundary-element solutions at a given stage of the deformation.

***Results:*** This method has been applied to a simple model of a silicon diaphragm, as shown schematically below. This structure was studied for different thicknesses, and the voltage-deflection behavior is also shown. These results show that for smaller voltages, the deflection, while nonlinear, behaves predictably. At larger voltages, the deflection becomes very large and an abrupt change is seen in the voltage deflection behavior. This critical voltage is generally referred to as the pull-in voltage for the diaphragm. Knowledge of this critical voltage is crucial for the design of MEMS structures that use an electrostatic actuation scheme.

***Significance:*** The ability to simulate the performance of electrostatically driven MEMS devices allows the designer to model the force-deflection behavior of these structures, as well as to determine the critical voltages at which the structure may become unstable. In addition, this code can be used to study the fundamental phenomena of elastic stability in the presence of coulombic interactions. This is an important problem in structural mechanics that, with the advent of micron-sized structures, has only recently been appreciated. The models developed with this code can be merged with circuit simulation to allow the designer to model the performance of the entire system.




*Micromachined silicon diaphragm*




*Voltage-deflection behavior for a silicon diaphragm*

# Semi-Analytical Finite-Element Modeling of Acceleration-Induced Frequency Change in SAW Resonators

J.T. Stewart
*Army Research Laboratory, Fort Monmouth, NJ*

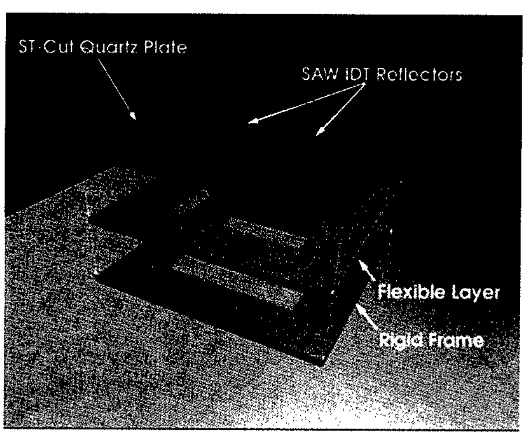
***Computer Resource:*** Cray C916 [CEWES MSRC]

***Research Objective:*** To develop a powerful and efficient modeling tool to aid in the design of low g-sensitivity surface acoustic wave (SAW) resonators for use in ultra stable oscillator applications such as airborne radar and missile guidance systems.

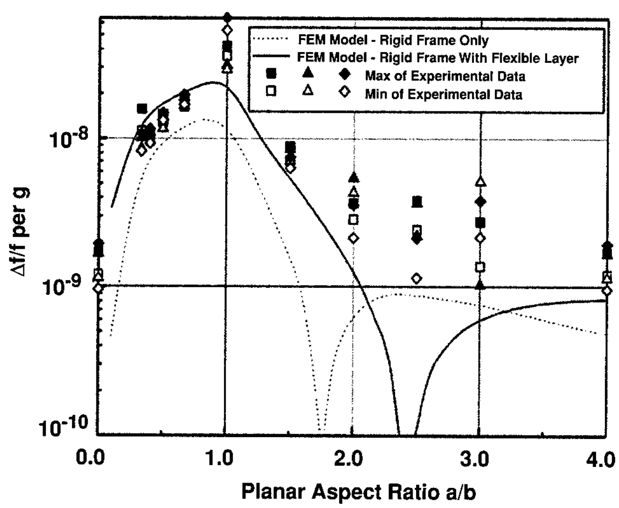
***Methodology:*** An analytical three-dimensional solution of a surface acoustic wave mode shape in a piezoelectric crystal is combined with a discrete finite-element solution to an acceleration-induced biasing state in a general perturbation theory to compute the g-force induced frequency shift in a SAW resonator. The method that has been developed consists of three basic steps: (1) the precise solution of the SAW mode shape for an arbitrary transverse harmonic in the transmission path and in the interdigitated transducer (IDT) reflector region; (2) an efficient and fast finite-element solution for the deformations in the crystal and its supporting structure under the action of acceleration; and (3) the numerical integration of the first perturbation of the eigenvalue to compute the frequency shift.

***Results:*** This code has been tested extensively against both classical solutions and actual experimental data with excellent results. Shown below is a comparison of results obtained using the modeling tool with experimental data obtained at ARL, Ft. Monmouth. In this experiment, a normal acceleration was applied to a SAW resonator mounted on a picture frame-type support consisting of a rigid layer and a soft layer of various dimensions. The experimental setup was then modeled with the design tool, and the results are plotted (smooth curves) along with the experimental data (scatter points). The modeling software is shown to predict the optimal planar aspect ratio (approximately 2.5) in accordance with the experimental data.

***Significance:*** The ability to simulate the acceleration sensitivity of crystal resonators with detailed modeling of the supporting structures is crucial to the design of high precision, ultra stable oscillators and other frequency control products. Components of this type are of fundamental importance to the development of weapons and communications systems that must be insensitive to vibration-induced noise. This tool allows the designer to determine optimal crystal cuts, resonator geometries, and support configurations for a given application. This modeling technology has the potential to greatly impact radar and electronic warfare systems such as Joint-STARS and ATRJ, and missile-guidance systems such as the patriot PAC III upgrade.




*General configuration for picture-frame-mounted SAW resonator*




*Comparison of modeled acceleration sensitivity with experimental data for picture-frame-mounted SAW resonator*

# Co-fired Ceramic Package for a Ka-Band MMIC Phase Shifter

J.-G. Yook and L.P.B. Katehi
*University of Michigan, Ann Arbor, MI*
*Army Research Office, RTP, NC*

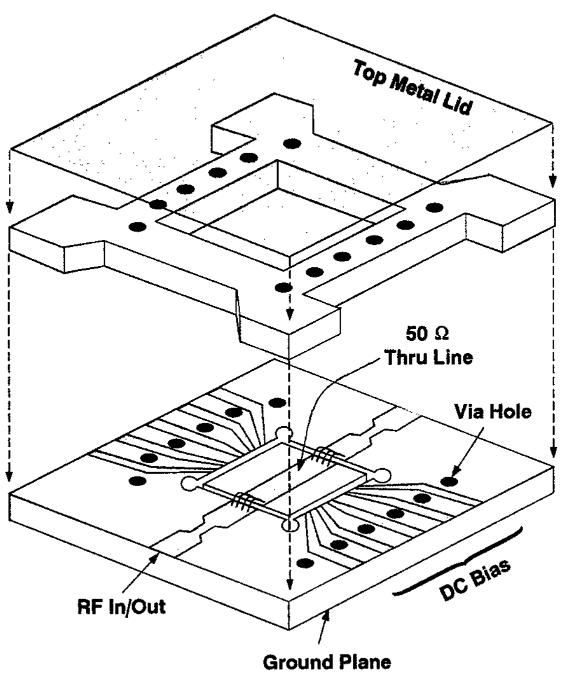
***Computer Resource:*** IBM SP2 [MHPCC DC]

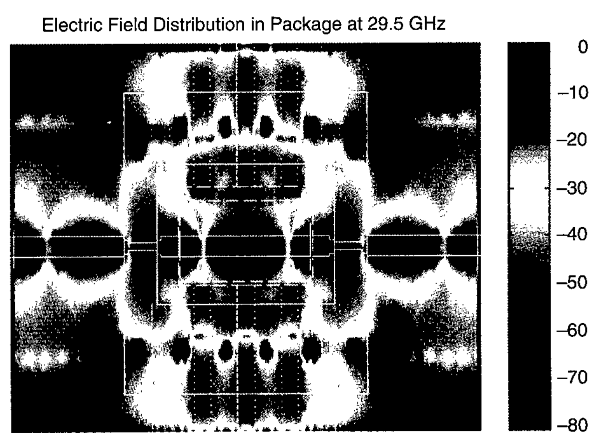
***Research Objective:*** To full-wave characterize microwave/millimeter wave packages for discrete MMIC (microwave monolithic integrated circuit) components. Although these packages are widely used in MMICs, their modeling has been limited by the large size and complexity of the problem, thus leading to long design cycles, low yield, and high cost.

***Methodology:*** To model the MMIC package, a full-wave finite-element (FEM) code has been parallelized on the distributed memory parallel computer. Task parallelization has been used because FEM is a frequency domain technique and, in these problems, each frequency point must be computed independently to obtain the complete package response over the desired frequency spectrum.

***Results:*** Preliminary results of the task parallelization strategy show linearly scalable performance improvement. This truly scalable parallel FEM code performs successfully as a result of the minimal communication overhead between the computing nodes and the fact that it is not subject to the bandwidth of the network or switches. The number of unknowns of the problem ranges from 150,000 to 200,000, and the global matrix equations are simultaneously built and solved at all frequency points within one hour. The same code would normally require 40 hours of processor time if it were run serially.

***Significance:*** Hermetic packages are frequently used in microwave integrated circuits to provide protection from a hostile environment, reduced electromagnetic interference, and minimal radiation leakage. A variety of packages based on a co-fired ceramic technology have been developed for use in high-frequency applications. This effort has provided, for the first time, a complete and accurate high-frequency characterization of an MMIC package and an understanding of its electromagnetic interference with the MMIC chip in the form of parasitic resonances.




*The 18-40 GHz MMIC package for phase shifter chip and electric field distribution in the package*

# W-Band Coplanar Waveguide Probe Structures

E.M. Tentzeris, J.-G. Yook, and L.P.B. Katehi
*University of Michigan, Ann Arbor, MI*
*Army Research Office, RTP, NC*

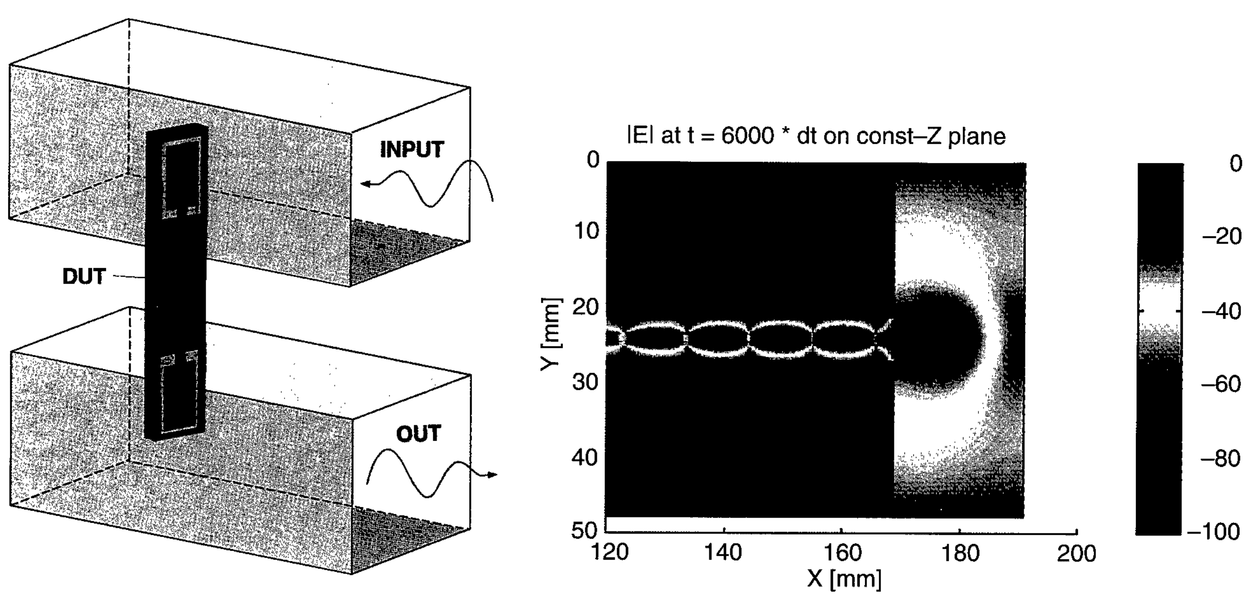
***Computer Resource:*** Convex SPP-1 [NCCOSC DC]

***Research Objective:*** To full-wave characterize W-band waveguide-probes, which are used either to probe modal propagation inside the waveguides or as active-element mounting structures. Significant attention is being devoted to the analysis and the design of these highly complex waveguide mounting structures.

***Methodology:*** The finite-difference time-domain (FDTD) technique has been used to calculate the S-parameters of a coplanar waveguide probe structure. The FDTD code has been parallelized on the Convex SPP-1 by using the "task parallelization" scheme.

***Results:*** A parametrical study has been performed for the probe dimensions to maximize, over the widest possible frequency range, the coupling between the probe and the waveguide. A waveguide absorber based on analytical Green's functions has been developed to minimize the reflections over a wide band of frequencies. As an application, a membrane coplanar waveguide probe has been characterized for a variety of geometrical parameters. The mesh size is $480 \times 477 \times 52$. This characterization would require about 250 hours of processor time if it were run on an HP 735 Workstation and 72 hours on the Cray C90 supercomputer. The parallelized version of the same program on the Convex SPP-1 requires about 31 hours of processor time for completion.

***Significance:*** This effort has allowed, for the first time, the complete and accurate high-frequency characterization of a W-band back-to-back probe configuration. Until recently, W-band probes for diode mounting or waveguide probing have been designed experimentally only through very long and costly design cycles.




*The membrane coplanar waveguide probe and the electric field distribution for the structure*

# Array-Enhanced Stochastic Resonance

A.R. Bulsara and M.E. Inchiosa
*Naval Command, Control and Ocean Surveillance Center, San Diego, CA*

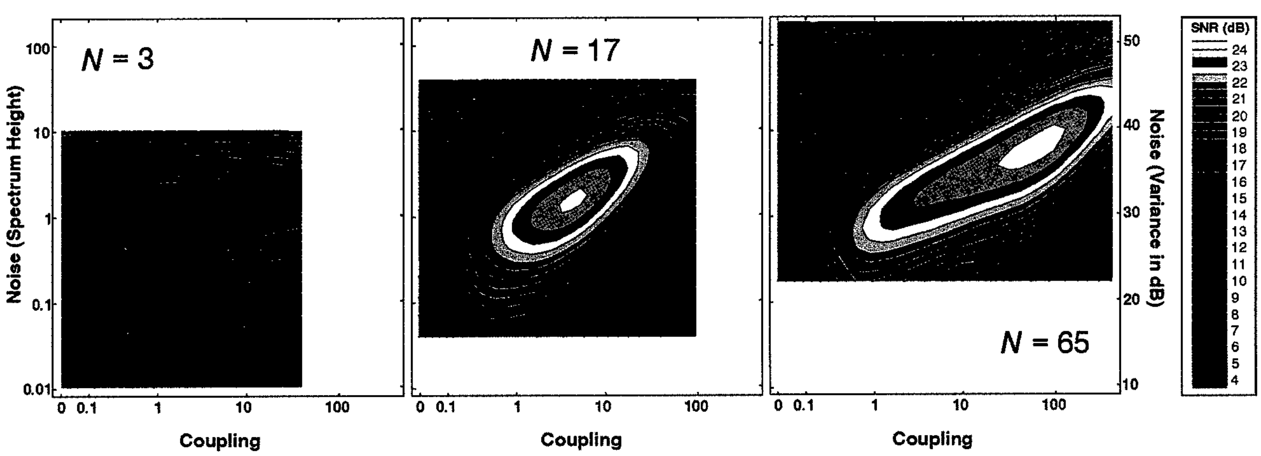
***Computer Resource:*** Intel Paragon [ASC MSRC and San Diego Supercomputer Center]

***Research Objective:*** Stochastic resonance (SR) is a peaking of response as noise power, rather than driving frequency, is varied. Theory predicts that coupling sensors to form arrays should enhance SR. High performance computing was used to determine how output signal-to-noise ratio (SNR), optimal noise power, and optimal coupling strength would scale with the number of array elements $N$, and to determine whether optimization of SNR implies optimization of signal detection statistics (probability of detection and probability of false alarm).

***Methodology:*** We numerically integrated coupled stochastic differential equations, performed fast Fourier transforms on the resulting time series, and produced power spectra from which we computed SNRs and signal detection statistics. We implemented two parallelization schemes on the Intel Paragon. For exploring parameter space, each Paragon node independently computes a result at a different parameter space point. For obtaining extremely well-averaged results at a single point in parameter space, all nodes operate with identical system parameters and independent noise realizations, afterwards performing a global sum operation to compute the averaged power spectrum. These schemes deliver essentially optimal parallel speedup.

***Results:*** For a linearly coupled chain of overdamped bistable oscillators, maximum output SNR indeed increases with $N$, rapidly at first, and then slowly. Also, optimizing output SNR does optimize signal detection performance. We required approximately 50,000 node hours (about 16 days using 128 Paragon nodes) to obtain these results.

***Significance:*** Array-enhanced SR can be exploited to design nonlinear sensors with improved signal detection performance in noisy environments. Under an SBIR Phase II grant, Quantum Magnetics, Inc., is currently studying the application of this technology to arrays of SQUID magnetometers envisioned for military (nonacoustic warfare, mine-hunting) and civilian (nondestructive evaluation, biomagnetics, geomagnetic remote sensing) applications. HPC simulations will be used in array design and optimization. Furthermore, we are studying SRs possible role in sensory neurons.




*Output SNR versus noise strength, coupling strength, and number of elements* N

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